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2011



Volume 18

Institute for Chemical Research
Kyoto University

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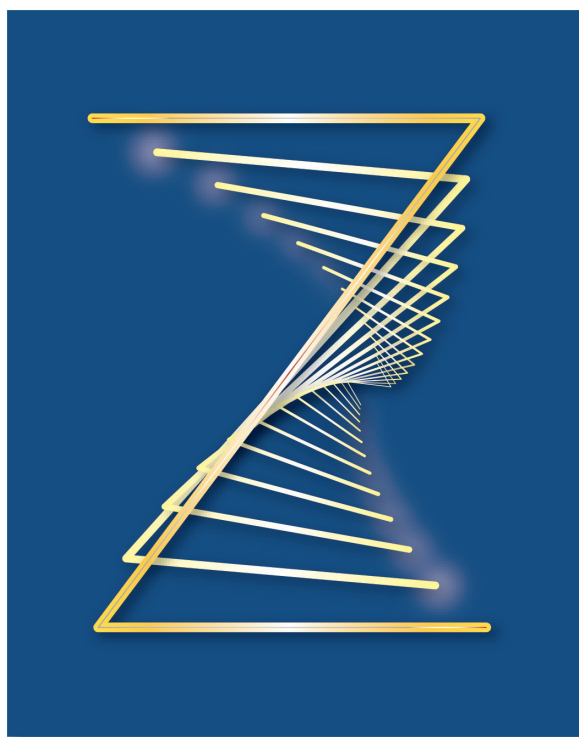
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**ICR
ANNUAL
REPORT
2011**



**Institute for Chemical Research
Kyoto University**
Volume 18



Preface

Before starting regular preface for the ICR Annual Report 2011, I wish to express our deepest sympathy to all those who have been affected by the destructive earthquake and tsunami which struck the Pacific coast of the northeastern region of Japan on March 11, 2011.

The Institute for Chemical Research (ICR) dates back to 1915, when the Specialized Center for Chemical Research was founded at the Faculty of Science, Kyoto Imperial University. The formation of the Specialized Center was greatly influenced by historical events. In 1910, Dr. Sahachiro Hata developed Salvarsan, a highly effective drug for syphilis, while conducting research with Dr. Paul Ehrlich. The effectiveness of this compound eventually became widely recognized, and its commercial production began in Germany. Japan was depending at that time on foreign deliveries of this drug, but the outbreak of World War I made further importation impossible. Forced by these unfortunate circumstances, the Japanese government requested the University of Tokyo and Kyoto University to produce Salvarsan. The fourth Chancellor of Kyoto University, Professor Mitsuru Kuhara, who also happened to be a chemist, received this request. Facilities for Salvarsan production were built with an investment of 20,000 yen, which is equivalent to about 200 million yen in today's market. Production went well, and as income was generated, faculty members with a passion for research in chemistry gathered from across the University to form the Specialized Center for Chemical Research, which was later expanded and renamed as the Institute for Chemical Research (ICR) in 1926. The newly established ICR soon began to produce outstanding research achievements: research on accelerators by Professor Bunsaku Arakatsu; research on synthesized petroleum oil production; and the development of vinylon, which was Japan's first synthetic fiber. Almost all professors at the institute, including the aforementioned, were also professors at the Faculty of Engineering or Science. However, over time, the University began to recognize the importance of having professors dedicated solely to the ICR in order to operate the ICR with a clear mission, as well as the importance of the institute's contribution in training researchers by providing guidance to graduate students. Thus, the ICR began accepting graduate students in 1962, and the reorganization in 1964 saw the installation of the research division system where each division was led by a dedicated professor. Since the founding of the ICR in 1926, our basic principle has been to excel in the investigation of basic principles of chemistry and their applications.

After several reorganizations, the ICR currently consists of the following five research divisions: Division of Synthetic Chemistry, Division of Materials Chemistry, Division of Biochemistry, Division of Environmental Chemistry, and Division of Multidisciplinary Chemistry complemented by the following three research centers: Advanced Research Center for Beam Science, International Research Center for Elements Science (IRCELS), and Bioinformatics Center. Today, the ICR spans 32 research fields (laboratories) with 102 faculty members and about 210 graduate students. Each laboratory belongs to one of the seven graduate schools which encompass science, engineering, agriculture, pharmaceutical science, medicine, informatics, and human and environmental studies. Our laboratories and the graduate schools work closely together to provide excellent graduate education. The ICR strives to be the "central research center in chemistry" by achieving outstanding results in chemistry and related fields, and

attracting motivated researchers in these fields. Chemistry is a fundamental science, which deals with materials, and its importance, including its contribution to physics and biology, cannot be overemphasized. One of our major strengths is our breadth and depth. In other words, the ICR is multidimensional, and is constantly widening and deepening its research activities. We intend to use our strengths to contribute to pioneering research, as well as to expand the boundaries of chemistry-related fields and to promote research collaborations, which are not easy in conventional graduate schools. Moreover, we aim to utilize our strengths as an outstanding center in education in order to produce excellent scientists and engineers who can actively contribute to our global society on the basis of their broad and profound perspective.

The ICR has executed three Global COE Programs in collaboration with the Graduate school of Engineering, the Graduate school of Science and the Graduate school of Informatics. These Programs include the "International Center for Integrated Research and Advanced Education in Material Science (2007-2011)" encompassing chemistry and materials science fields, the "Center of Excellence for Education and Research on Photonics and Electronics Science and Engineering (2007-2011)" involving information science, electrical engineering, and electronics fields, and "The Next Generation of Physics, Spun from Universality & Emergence Developing Independent Researchers to Explore New Frontiers (2008-2012)" covering physics, astronomy, and materials chemistry fields.

In addition, the ICR is making enthusiastic contribution to the MEXT Project of Integrated Research on Chemical Synthesis (2010-2016)", in collaboration with the Catalysis Research Center at Hokkaido University, the Research Center for Materials Science at Nagoya University and the Institute for Materials Chemistry and Engineering at Kyushu University. This is the second stage of the project supported by MEXT through the Research and Education Funding for Inter-University Research Projects. Furthermore, the ICR is currently collaborating with domestic/oversea universities and research organizations (with 54 official international collaboration agreements) and has been functioning as a Joint Usage/Research Center supported by MEXT, "Frontier/ Interdisciplinary Research Core in ICR for Deepening Investigation and Promoting Cooperation in Chemistry-Oriented Fields" (since 2010). The strong network of collaborations constructed inside and outside the ICR ensures that our institute serves as the center of global research propellers in chemistry-oriented fields. We are happy that, the recent years have seen the successful construction of a new lecture hall "Uji Obaku Plaza" (2009) and the completion of the four year long earthquake-proof renovation of the main buildings in the Uji campus (2010). With these highly improved research/education facilities, we are bringing ourselves closer to attain our founding philosophy. Thus, we respectfully request your continued support and encouragement.

January 2012

A handwritten signature in black ink, reading "N. Tokitoh". The signature is fluid and cursive.

TOKITOH, Norihiro
Director

ICR News 2011

Completion of Seismic Retrofit for the Main Building in Uji Campus



Main Building of Uji Campus

■ Prof WATANABE, Hiroshi (Vice-Director of ICR)

The main building in Uji Campus, where many (~70%) research divisions of the Institute for Chemical Research (ICR) are accommodated, was constructed in 1968. As this building did not meet the current quake-resistance standards (and had aged significantly), a seismic retrofit was urgently required. Thus, the institutes/departments in Uji campus cooperated to negotiate with the university executive office and an extensive seismic retrofit was made during the period of 2007-2010. A budget shortfall from the executive office was overcome by, for example, minimization of the move/evacuation of laboratories during this period, leading to the satisfactory completion of the enterprise. This retrofit not only allowed the main building to meet the quake-resistance standards but also resulted in improvements of the facilities in Uji campus through

centralization of the radioisotope laboratories, redesigning of the Uji library, and introduction of new common spaces in the campus (such as a relaxation room for women, shower booths, and so on). Furthermore, on the occasion of the retrofit, ICR spent its own budget to increase the laboratory area and upgrade the research facilities. In particular, new research laboratories equipped with advanced instruments, *e.g.*, 800 MHz NMR, have been assigned as open laboratories of the ICR Joint Usage/Research Center (ICR-JURC) approved by MEXT as of 2010, thereby serving as a strong base for enhanced collaboration between ICR and other universities/research institutes as well as among the ICR faculty members. Thus, the effort of ICR for the seismic retrofit was rewarded by many infrastructure improvements to the facilities at ICR.



Uji Radioisotope Laboratory



Uji Library



800 MHz NMR



Relaxation Room for Women

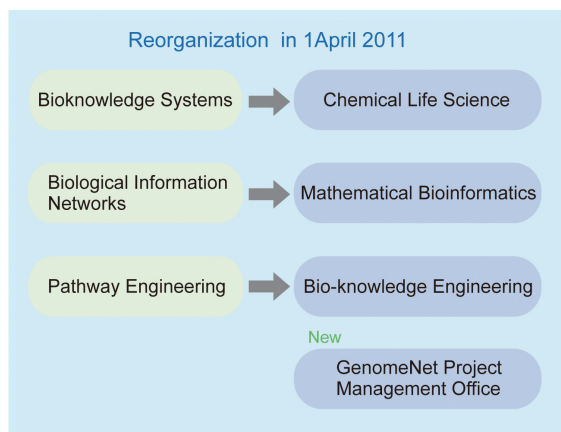
Bioinformatics Center's New Restructuring and 10 Year Anniversary Symposium

In April 2011, 10 years after the establishment, the Bioinformatics Center in the Institute for Chemical Research (ICR) conducted organizational restructuring resulting in the creation of three new laboratories, named, Chemical Life Science, Mathematical Bioinformatics and Bio-knowledge Engineering. Additionally, an administrative office has been created called the GenomeNet project management office which will be responsible for maintaining the high-end supercomputers in ICR and continuation of the GenomeNet database service. Furthermore, as a celebration of the 10 year anniversary of the Bioinformatics Center, on the 29th of August 2011, a symposium named "ICR Symposium to Celebrate the Bioinformatics Center's 10 Year Anniversary and Restructuring" was held, having invited nine outstandingly working researchers in Bioinformatics for speakers and received more than 30 submissions for poster presentations. The main objective of the symposium was to have a view to future directions with our newly restructured center.

■ Prof MAMITSUKA, Hiroshi
(Director of Bioinformatics Center)



■ <http://www.bic.kyoto-u.ac.jp/pathway/bic10years/> (for details of the symposium)



New Organization of Bioinformatics Center



Participants of 10 Year Anniversary Symposium



Lecture of Prof KANEHISA, Minoru



Symposium in Kihada Hall, Uji Obaku Plaza



Poster Session

Inauguration of ICR Program Supporting Research Stay of Young Researchers at/from Oversea Institutes

■ Prof WATANABE, Hiroshi (Vice-Director of ICR)

In September 2011, the Institute for Chemical Research (ICR) inaugurated its own program that supports, both financially and academically, the research stay of young researchers of ICR (including graduate students) at overseas institutes and the stay at ICR for young researchers from overseas institutes, for periods of 2-12 weeks and 3-12 weeks, respectively. This program calls for/adopts the application on a quarterly basis and further accepts occasional applications on urgency, thereby offering very flexible/agile opportunities not available in other programs so far.

This ICR program is applied mainly to the research stay at/from overseas institutes that have concluded the Memorandum of Agreement (MOU) for international collaboration with ICR (currently 54 institutes), but also welcomes the stay at/from other overseas institutes. Within 3 months after the start of the program, it has already supported six young researchers of ICR and one from Europe. The program will continue to actively support young researchers in coming fiscal years.

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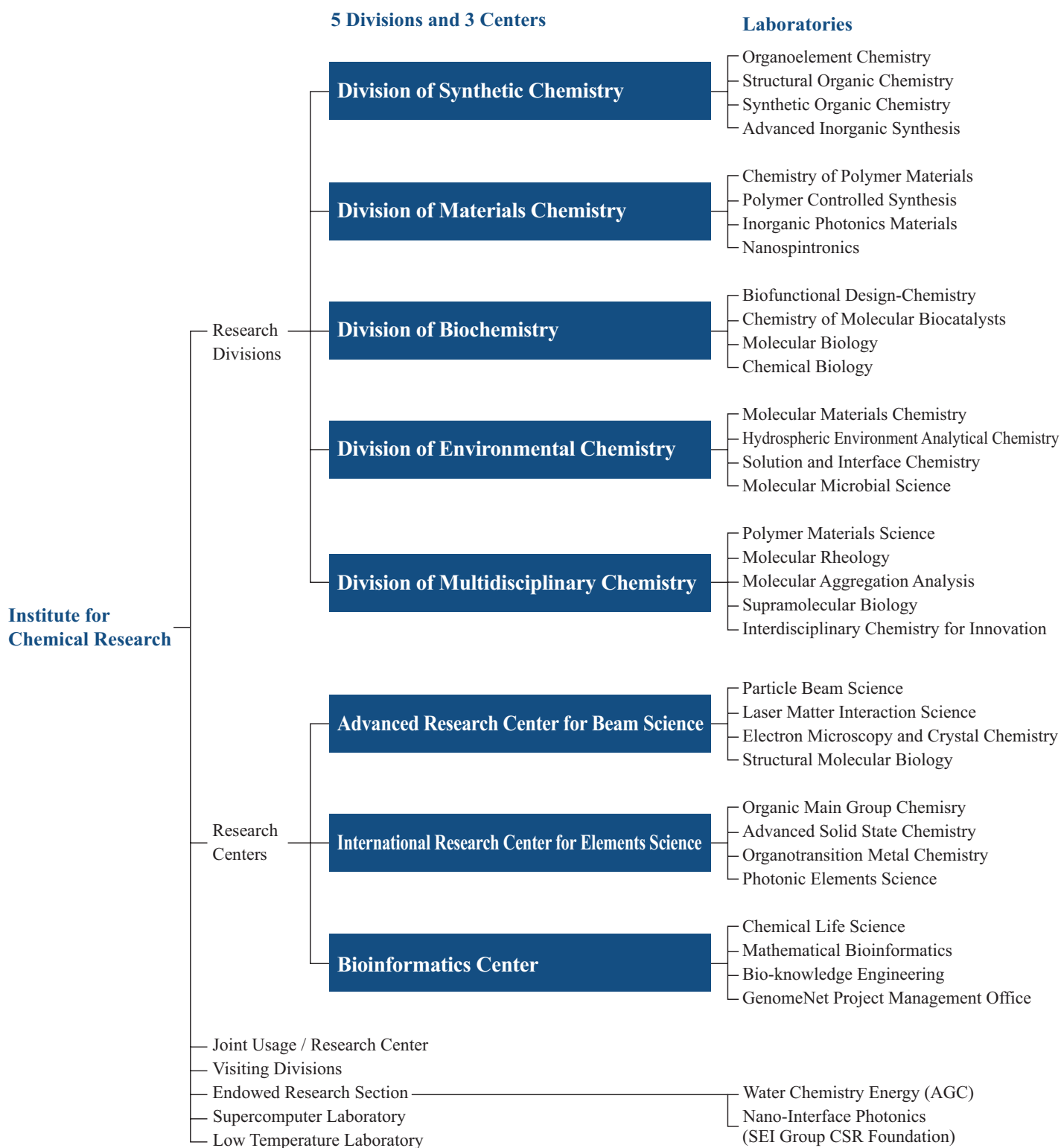
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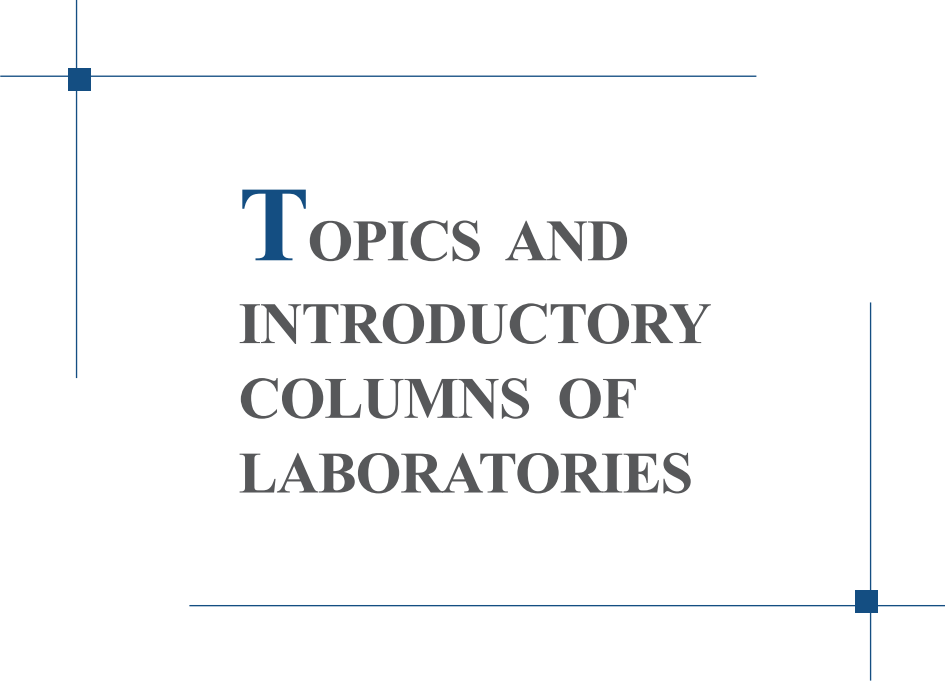
Abbreviations used in the columns

Prof Em	Professor Emeritus	SPD	Special Post-Doctoral Research Fellow
Prof	Professor		
Vis Prof	Visiting Professor	PD	Post-Doctoral Research Fellow
Assoc Prof	Associate Professor	Res	Researcher
Vis Assoc Prof	Visiting Associate Professor	A Res	Assistant Researcher
Lect	Lecturer	Proj Res	Project Researcher
Assist Prof	Assistant Professor	RF	Research Fellow
Program-Specific	Assoc Prof	D 1 ~ 3	Doctoral Course (Program) 1 ~ 3
	Program-Specific Associate Professor	M1 ~ 2	Master's Course (Program) 1 ~ 2
	Professor	RS	Research Student
Program-Specific	Assist Prof	UG	Undergraduate Student
	Program-Specific Assistant Professor	D Sc	Doctor of Science
	Professor	D Eng	Doctor of Engineering
Vis Assist Prof	Visiting Assistant Professor	D Agr	Doctor of Agricultural Science
Program-Specific	Res	D Pharm Sc	Doctor of Pharmaceutical Science
	Program-Specific Researcher	D Med Sc	Doctor of Medical Science
Res Associate	Research Associate	D Inf	Doctor of Informatics
Techn	Technician	Ph D	Doctor of Philosophy
Guest Scholar	Guest Scholar	(pt)	part-time
Guest Res Assoc	Guest Research Associate	iCeMS	Institute for Integrated Cell-Material Sciences



ORGANIZATION





TOPICS AND
INTRODUCTORY
COLUMNS OF
LABORATORIES

Division of Synthetic Chemistry – Organoelement Chemistry –

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



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Prof JURKSCHAT, Klaus

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Department of Organic Chemistry, Maria Curie-Skłodowska University, Poland, 27–29 June

Institut für Chemie, Technische Universität Berlin, Germany, 15 September

Department of Chemistry, Centre for Advanced Solar Materials, University of Calgary, Canada, 15–16 November

Lehrstuhl für Anorganische Chemie II, Technische Universität Dortmund, Germany, 5–6 December

Scope of Research

Organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of “dreams” for organic chemists. Our main research interest is the elucidation of the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting and important from the standpoints of not only fundamental chemistry but also opening the way to more extensive application of main group chemistry.

Selected Publications

Tsurusaki, A.; Sasamori, T.; Wakamiya, A.; Yamaguchi, S.; Nagura, K.; Irle, S.; Tokitoh, N., Synthesis of 1-Phospha-2-boraacenaphthenes: Reductive 1,2-Aryl Migration of 1-Diarylboryl-8-dichlorophosphinonaphthalenes, *Angew. Chem. Int. Ed.*, **50**, 10940–10943 (2011).

Sugamata, K.; Sasamori, T.; Tokitoh, N., Fluorination Reaction of a Ditelluride Bearing Bulky Aryl Substituents: Formation of Mixed-Valent $\text{Te}^{\text{IV}}\text{-Te}^{\text{II}}$ Ditelluride Difluoride, *Chem. Asian J.*, **6**, 2301–2303 (2011).

KEYWORDS

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

LiBr-Assisted Generation of a Silylenoid from 1,2-Dibromodisilene

Silylenoids (R_2SiMX) are the silicon analogues of carbenoids, where X denotes a leaving group (e.g., halogen or alkoxy) and M is a metal atom. Silylenoids have comparable reactivity to silylenes ($R_2Si:$) and react with both electrophiles and nucleophiles. During the course of our studies on 1,2-diaryl-1,2-dibromodisilene **1**, we found the evidence for the LiBr-assisted generation of silylenoid **2** and/or silylene **3** from **1**. This work provides a unique method to the *in situ* generation of silylenes from disilenes. It is noteworthy that the reaction products (e.g., compounds **4-6**) from this study still contain a Si–Br bond, which can be exploited in subsequent reactions.

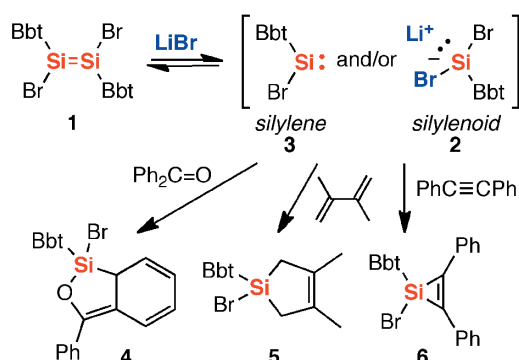
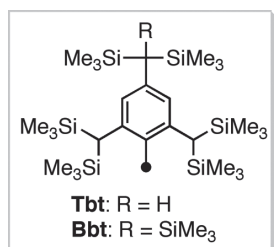


Figure 1. Generation of silylenoid **2**.

1-Phospha-2-boraacenaphthenes

Chemistry of organic π -electron conjugated molecules bearing several main group elements, especially group 13 and/or 15 elements, in their backbones have attracted much attention in recent years from the viewpoint of material science, because group 13 and 15 elements should drastically change the HOMO and LUMO levels of the π -conjugated systems. We have achieved the synthesis of 1,2-diaryl-1-phospha-2-boraacenaphthenes **7**, which are new members of heterocyclic compounds containing a P–B bond. Compounds **7** were synthesized as orange crystals by the reduction of 1-diarylboryl-8-dichlorophosphenaphthalene via a unique intramolecular migration of the aryl group from the boron to phosphorus atoms. Furthermore, **7** showed orange fluorescence with a large Stokes shift. Both experimental and theoretical results on **7** revealed the significant interaction between a P–B bond and a naphthyl unit.

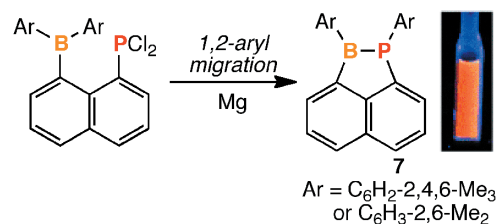


Figure 2. Syntheses of 1-Phospha-2-boraacenaphthenes.

Formation of Te(IV)–Te(II) Mixed-valent Ditelluride Difluoride

Because of their rapid disproportionation reactions, monoorganotellurium(II) monohalides, RTeX, are very unstable and difficult to isolate. Above all, monoorganotellurium(II) monofluorides, RTeF, are extremely unstable compounds, and no organotellurium(II) fluorides kinetically stabilized by bulky organic substituents have been reported, even though there have been a few stable examples of monoorganotellurium(II) halides (Cl, Br, I). We have reported the synthesis and isolation of monoorganotellurium(II) halides kinetically stabilized by a Bbt group. It was found that BbtTeX (X = Cl, Br, I) keep their monomeric structures both in solution and in the solid state. In the case of X = F, in contrast, not the expected BbtTeF but a novel species of a Te(IV)–Te(II) mixed-valent ditelluride difluoride, BbtTe(F)₂–TeBbt (**9**), was obtained as a stable compound. One of the tellurium atoms exhibits pseudo trigonal bipyramidal geometry as a hypervalent compound, and the two fluorine atoms occupy the apical positions. The NMR study at variable temperature showed its high thermal stability with keeping the mixed-valent structure in solution.

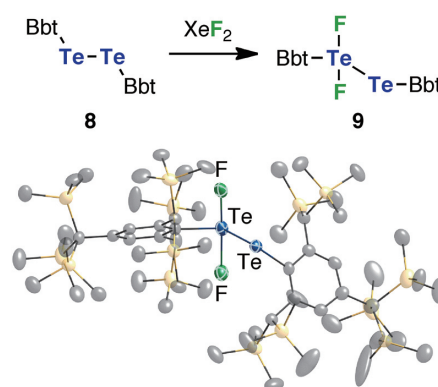


Figure 3. Synthesis and Structure of Mixed-valent Ditelluride Difluoride.

Division of Synthetic Chemistry – Structural Organic Chemistry –

<http://www.scl.kyoto-u.ac.jp/-kouzou/index.html>



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(D Eng)



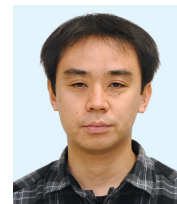
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Prof MARGETIĆ, Davor

Prof LIU, Shih-Yuan

Prof WU, Jishan

School of Physics, Queen Mary, University of London, U.K., 18 April

Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Germany, 8 October

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Croatia,
7 December

Department of Chemistry, University of Oregon, U.S.A., 12 December

Department of Chemistry, National University of Singapore, Singapore, 22 December

Scope of Research

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

Selected Publications

Morinaka, Y.; Tanabe, F.; Murata, M.; Murata, Y.; Komatsu, K., Rational Synthesis, Enrichment, and ^{13}C NMR Spectra of Endohedral C_{60} and C_{70} Encapsulating a Helium Atom, *Chem. Commun.*, **46**, 4532-4534 (2010).

Job, A.; Wakamiya, A.; Kehr, G.; Erker, G.; Yamaguchi, S., Electronic Tuning of Thiazolyl-Capped π -Conjugated Compounds via a Coordination/Cyclization Protocol with $B(C_6F_5)_3$, *Org. Lett.*, **12**, 5470-5473 (2010).

Murata, M.; Morinaka, Y.; Murata, Y.; Yoshikawa, O.; Sagawa, T.; Yoshikawa, S., Modification of σ -Framework of [60]Fullerene for Bulk-heterojunction Solar Cells, *Chem. Commun.*, **47**, 7335-7337 (2011).

Frunzi, M.; Jockusch, S.; Chen, J. Y. -C.; Calderon, R. K.; Lei, X.; Murata, Y.; Komatsu, K.; Guldi, D. M.; Lawler, R. G.; Turro, N. J., A Photochemical On-Off Switch for Tuning the Equilibrium Mixture of H_2 Nuclear Spin Isomers as a Function of Temperature, *J. Am. Chem. Soc.*, **133**, 14232-14235 (2011).

Kurotobi, K.; Murata, Y., A Single Molecule of Water Encapsulated in Fullerene C_{60} , *Science*, **333**, 613-616 (2011).



KEYWORDS

π -Conjugated Systems

Open-Cage Fullerenes

Endohedral Fullerenes

Functional Dyes

Organic Solar Cell

A Single Molecule of Water Encapsulated in Fullerene C₆₀

The C₆₀ encapsulating a water described here is a totally new member of endohedral fullerenes produced only by the present method. In contrast with the maturity of the science of empty fullerenes, research on endohedral fullerenes has not been fully developed in spite of their potentiality for various applications. This is ascribed to severe limitations in their production and isolation with high purity even in mg quantities. Their current production relying on physical method needs to be improved. We have succeeded in the macroscopic production of endohedral C₆₀ encapsulating a water molecule in 100%, by a new approach using the methodology of organic synthesis with the dynamic control of the opening-size on an open-cage fullerene derivative. This result indicates that currently employed physical method for the production of endohedral fullerenes, which relies on accidental and uncontrollable self-assembly of atoms, can be replaced by the fully controlled and rational synthetic method of much higher efficiency.

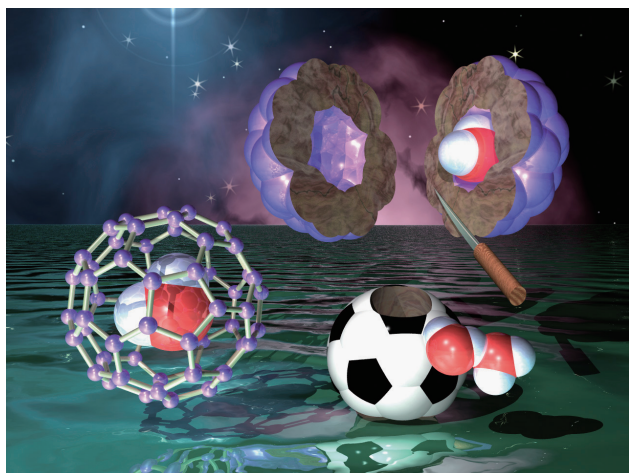


Figure 1. Molecular structure of H₂O@C₆₀.

Modification of σ -Framework of C₆₀ for Bulk-heterojunction Solar Cells

The organic thin-film photovoltaic devices, so called bulk-heterojunction (BHJ) solar cell, possesses a high potentiality as a renewable energy source because of its easy fabrication through solution process, flexibility, and large area application. In the BHJ cells [60]Fullerene derivatives have occupied a dominant position as an n-type organic semiconductor. However, much effort has so far been focused on developments of the donor polymer, while those of n-type materials remain untapped although some simple addition reactions to the surface of the C₆₀ cage are used. In this study, we have clearly demonstrated that the skeletal-modification of C₆₀ can be used to control the electronic properties and, thus, can be a promising avenue toward the novel acceptor materials for the BHJ solar cells. The device using the skeletally-modified C₆₀ derivative marked excellent open-circuit voltage (V_{oc} =0.74 V) and power conversion efficiency

(η_e =3.1%) with reference to the device using the benchmark acceptor PCBM (V_{oc} =0.60 V, η_e =3.1%).

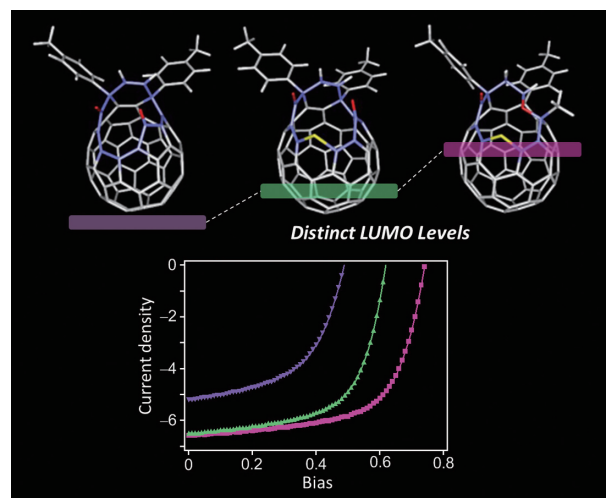


Figure 2. Open-cage C₆₀ derivatives and their application to the bulk-heterojunction solar cells.

Planarized Triaryboranes as Boron-embedded 2D π Scaffolds

Electron-accepting π -conjugated skeletons have long been sought for development of excellent n-type semiconducting materials in organic electronics. Incorporation of electron-deficient boron atoms into a two-dimensionally expanded π -skeleton should be a promising strategy to this end. As a simple example, we now synthesize triphenylborane and its diboron homologue that are completely planarized with methylene tethers. In contrast to the conventional concept for the kinetic stabilization of boron-containing materials by bulky substituents, the produced compounds show high stability toward air and moisture, and even toward Lewis acidic amines despite the absence of steric protection around the boron moiety. These results should give a new paradigm for the stabilization of the tri-coordinate boron-containing materials. A notable advantage to embed the boron atoms into the π -skeleton is to allow us the structural and properties modification based on the coordination number change of the boron atoms. Indeed, upon treatment with fluoride ions, the triphenylborane derivatives undergo the plane-to-bowl conversion in a controlled manner.

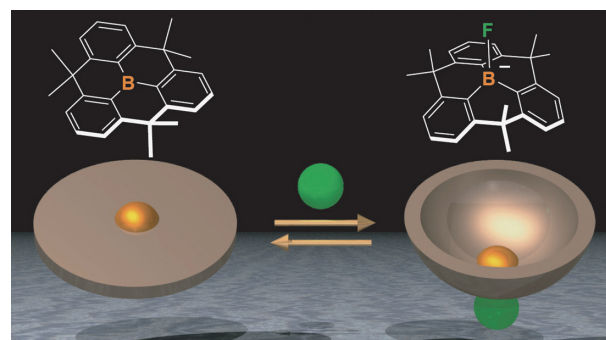


Figure 3. A controlled plane-to-bowl conversion based on the coordination number change of the boron atom.

Division of Synthetic Chemistry – Synthetic Organic Chemistry –

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Scope of Research

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

KEYWORDS

Organocatalysis Unusual Amino Acid
Regioselective Functionalization Molecular Recognition
Dynamic Chirality



Selected Publications

- Kawabata, T.; Matsuda, S.; Kawakami, S.; Monguchi, D.; Moriyama, K., Stereochemical Diversity in Asymmetric Cyclization via Memory of Chirality, *J. Am. Chem. Soc.*, **128**, 15394-15395 (2006).
- Kawabata, T.; Muramatsu, W.; Nishio, T.; Shibata, T.; Schedel, H., A Catalytic One-Step Process for the Chemo- and Regioselective Acylation of Monosaccharides, *J. Am. Chem. Soc.*, **129**, 12890-12895 (2007).
- Kawabata, T.; Moriyama, K.; Kawakami, S.; Tsubaki, K., Powdered KOH in DMSO: An Efficient Base for Asymmetric Cyclization via Memory of Chirality at Ambient Temperature, *J. Am. Chem. Soc.*, **130**, 4153-4157 (2008).
- Kawabata, T.; Jiang, C.; Hayashi, K.; Tsubaki, K.; Yoshimura, T.; Majumdar, S.; Sasamori, T.; Tokitoh, N., Axially Chiral Binaphthyl Surrogates with an Inner N-H-N Hydrogen Bond, *J. Am. Chem. Soc.*, **131**, 54-55 (2009).
- Muramatsu, W.; Mishiro, K.; Ueda, Y.; Furuta, T.; Kawabata, T., Perfectly Regioselective and Sequential Protection of Glucopyranosides, *Eur. J. Org. Chem.*, **5**, 827-831 (2010).
- Yoshida, K.; Furuta, T.; Kawabata, T., Organocatalytic Chemoselective Monoacylation of 1,n-Linear Diol, *Angew. Chem. Int. Ed.*, **50**, 4888-4892 (2011).

Organocatalytic Chemoselective Monoacylation of 1,*n*-Linear Diol

Selective monoacylation of 1,*n*-linear diols seems simple molecular transformation, however, it is still a challenging subject in current organic synthesis because overacylation is usually unavoidable. Since the steric environments of the free OHs in diol **2** are similar to those of a free OH in monool **3** (Figure 1d), strategy for monoacylation based on conventional steric repulsive interaction is not effective, especially in the cases of long-chain diols. We describe here chemoselective monoacylation of **2** by organocatalytic discrimination of **2** from **3** via molecular recognition. In the presence of catalyst **1**, exclusive or predominant monoacylation of 1,*n*-linear diols took place when the chain length of linear diols is equal to or shorter than five (Figure 1b). In sharp contrast to the acylation catalyzed by **1**, random acylation of linear diols was observed in DMAP-catalysed acylation, independently from the chain length of diols (mono/diacylate=0.6~3.1, Figure 1c). Acylation catalyzed by **1** is diol-selective and chain-length-selective (Figures 1d,e). The relative rate of the acylation between 1,5-pentanediol (**2**) and its monoacylate (**3**) was found to be 113, while that of DMAP-catalyzed acylation was 1.0 (Figure 1d). The high diol-selectivity observed in the acylation catalyzed by **1** seems to be the origin of the high selectivity for monoacylation of linear

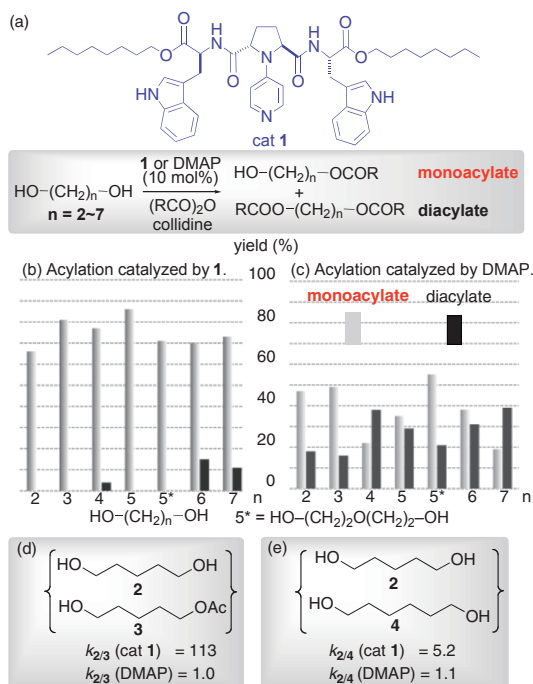


Figure 1. (a) Acylation of 1,*n*-linear diols catalyzed by **1** or DMAP. Ratios of the mono-/diacylate in the acylation of catalyzed by **1** (b) and DMAP (c). The relative rate of acylation between **2** and **3** (d), and between **2** and **4** (e).

diols. Catalyst **1** appears to discriminate the chain length of the diols on acylation. 1,5-Pentanediol (**2**) was found to be acylated 5.2 times faster than its one-carbon-longer analogue, 1,6-hexanediol (**4**) (Figure 1e).

Asymmetric Intermolecular Conjugate Addition of Axially Chiral Enolates: Total Synthesis of Manzacidin A

Unusual amino acids and their analogues have attracted considerable attention because of their potential utilities in the fields of natural product syntheses and medicinal chemistry. We developed a synthetic method of α,δ -diaminoglutaric acid derivatives via intermolecular conjugate addition of chiral enolates generated from readily available α -amino acids. In this reaction, asymmetric nucleophilic addition of chiral enolates **A** (blue thick arrow) competes racemization of axially chiral enolate **A** by C-N bond rotation {red arrow, half-life of racemization of **A** (R=Me)=1 h at -78°C }. The highly enantioselective intermolecular conjugate addition of the enolates has been achieved by use of highly reactive Michael acceptor **6** as well as elaboration of the experimental procedure. Slow addition of potassium hexamethyldisilazide (KHMDs) in THF to a mixture of **5** (R=Me) and **6** in DMF at -78°C gave a 1:1 diastereomeric mixture of **7** (R=Me) in a quantitative combined yield and in 97% ee and 97% ee, respectively. The conjugate addition of enolate **A** was found to proceed with a retention of configuration at the newly formed tetrasubstituted stereocenter. This method is well applicable for other α -amino acid derivatives such as phenylalanine derivative **5** (R=CH₂Ph) and methionine derivative **5** (R=CH₂CH₂SMe). One of the diastereomer of **7** (R=Me, 97% ee) was successfully transformed to marine natural product manzacidin A. In this transformation, all of the carbon-nitrogen framework obtained by the asymmetric conjugate addition are incorporated in the structure of manzacidin A (shown in blue in Figure 2, The MOM group is utilized as a methylene unit between two nitrogen atoms).

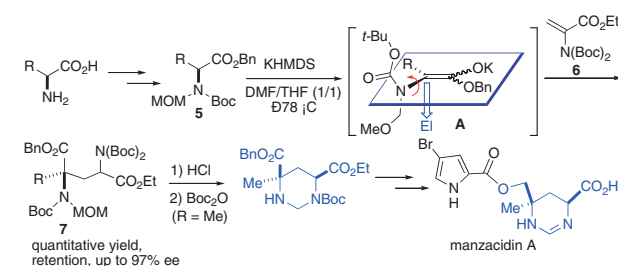


Figure 2. Asymmetric intermolecular conjugate addition of chiral enolates **A** derived from amino acid derivatives **5** and total synthesis of manzacidin A from the adduct **7**.

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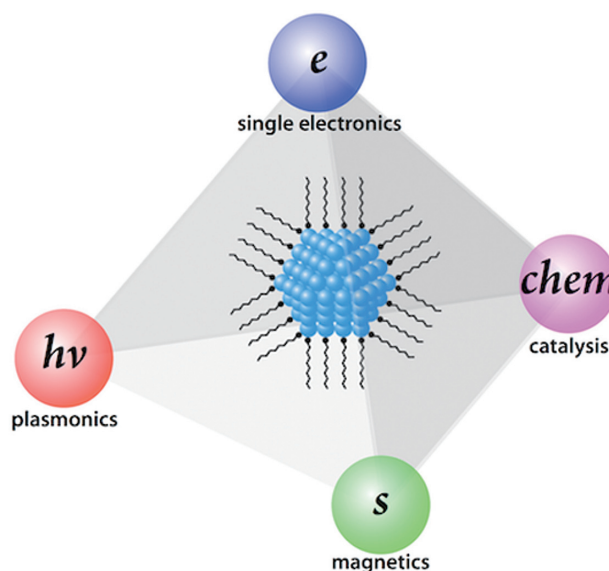
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Scope of Research

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 their properties, such as electron confinement, carrier oscillation, spin, and catalysis. These high quality inorganic nanoparticles are applied to both high-performance nanodevices (single electron transistor, plasmon waveguide, nanocomposite magnet) and photo-energy conversion materials (overall water splitting, solar cell).



KEYWORDS

Inorganic Nanoparticles
Single Electronics
Plasmonics
Nanocomposite Magnet
Overall Water Splitting

Selected Publications

- Saruyama, M.; So, Y. -G.; Kimoto, K.; Taguchi, S.; Kanemitsu, Y.; Teranishi, T., Spontaneous Formation of Wurtzite-CdS/Zincblende-CdTe Heterodimers through a Partial Anion Exchange Reaction, *J. Am. Chem. Soc.*, **133**, 17598-17601 (2011).
- He, C. -L.; Chen, H. -Y.; Wang, C. -Y.; Lin, M. -H.; Mitsui, D.; Eguchi, M.; Teranishi, T.; Gwo, S., Far-Field Optical Imaging of a Linear Array of Coupled Gold Nanocubes at Visible Wavelengths: Direct Visualization of Dark Plasmon Modes, *ACS Nano*, **5**, 8223-8229 (2011).
- Saruyama, M.; Kanehara, M.; Teranishi, T., Drastic Structural Transformation of Cadmium Chalcogenide Nanoparticles Using Chloride Ions and Surfactants, *J. Am. Chem. Soc.*, **132**, 3280-3282 (2010).
- Kanehara, M.; Koike, H.; Yoshinaga, T.; Teranishi, T., Indium Tin Oxide Nanoparticles with Compositionally Tunable Surface Plasmon Resonance Frequencies in the Near IR Region, *J. Am. Chem. Soc.*, **131**, 17736-17737 (2009).
- Li, C.; Sato, R.; Kanehara, M.; Zeng, H.; Bando, Y.; Teranishi, T., Controllable Polyol Synthesis of Uniform Palladium Icosahedra: Effect of Twinned Structure on Deformation of Crystalline Lattices, *Angew. Chem. Int. Ed.*, **48**, 6883-6887 (2009).

Charge Separation in Type-II CdS/CdTe Heterodimers Formed by Anion Exchange Reaction

Heterostructured nanoparticles (NPs), in which two or more distinct inorganic materials are connected together, are expected to provide new ways to manipulate wave functions, plasmon resonances, and spin. In semiconductor heterostructures, the choice of semiconductor materials allows control of the manner of confinement of the electron and hole wave functions in NPs. Type-II heterostructured NPs with a staggered alignment of band edges at the heterointerface can promote spatial charge separation of the electron and hole in different parts of the heterostructure for photocatalytic and photovoltaic applications.

The CdS/CdTe combination was chosen because this heterointerface forms a type-II band-edge alignment. The thermodynamically stable phases of CdS and CdTe crystals are wurtzite (*w*) and zinc blende (*zb*), respectively, and large strain at the heterointerface should induce spontaneous phase segregation. The anion exchange reaction proceeded smoothly to give anisotropically phase-segregated CdS/CdTe heterodimers with one heterointerface as an intermediate during formation of the completely exchanged product, CdTe NPs. Spontaneous formation of CdS/CdTe heterodimers took place because of the strain relaxation of the different crystallographic orientations of the *w*-CdS and *zb*-CdTe phases. As shown in Figure 1, atomic-resolution high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) observations revealed that the heterointerface was *w*-CdS (0001)/*zb*-CdTe ($\bar{1}\bar{1}\bar{1}$). Transient absorption spectroscopy demonstrated that photoinduced onedirectional charge separation occurred in CdS/CdTe heterodimers because of the type-II band-edge alignment with one heterointerface.

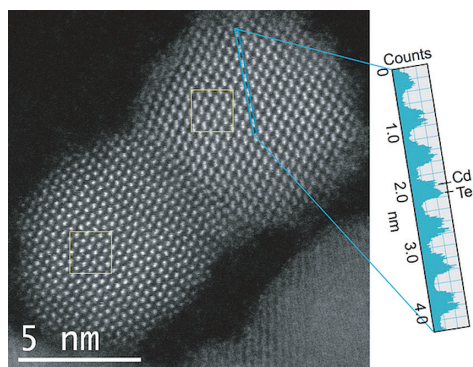


Figure 1. Atomic-resolution HAADF-STEM image of a single *w*-CdS/*zb*-CdTe heterodimer.

Dark Plasmon Propagation in Linear Array of Coupled Gold Nanocubes

Localized surface plasmon polaritons, which are referred to simply as localized surface plasmons, are collective electron oscillations in conductive NPs that are excited by incident light waves. Recently, the concept of optical nanoantennas based on plasmonic metal nanostructures has emerged as a promising route to realize optics and photonics far beyond the diffraction limit. In its inception, plasmonic nanoantennas composed of single metallic nanorods or nanoparticles were proposed as subwavelength receivers and/or transmitters of optical fields.

Recently, we have developed an alternative nanomanipulation technique for assembly of gold octahedron nanocrystal dimers with precisely controlled interoctahedron nanogaps. By studying the gold nanocube chains precisely assembled with tunable intercube separations, the fundamental plasmonic effects can be revealed in detail under well-prepared experimental settings, such as the number and spacing of nanocubes as well as the incident light direction and scattering light polarization. Using these chains, we were able to measure the dispersion relations of coupled plasmons with respect to the number of composing nanocubes and the intercube distance. In contrast to the existing results in the literature, we found that the plasmon coupling in gold nanocrystal structures could extend over a long spatial range (a few micrometers), resulting from the superior plasmonic properties of gold nanocubes, as shown in Figure 2. In addition, we confirmed that plasmonic waveguiding could only occur when the intercube distance is very small (much smaller than the nanocube feature size; under near-field plasmon coupling conditions).

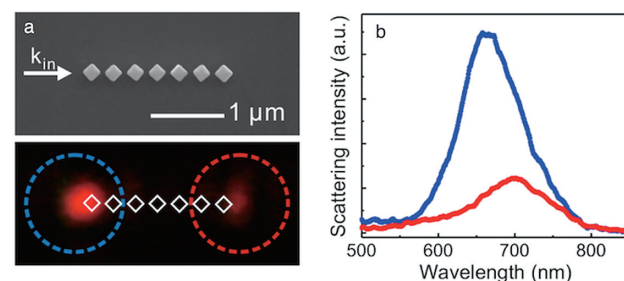


Figure 2. (a) FE-SEM image showing a chain composed of 7 uniformly spaced nanocubes (intercube tip-to-tip separation: 70 ± 5 nm). (b) Scattering spectra acquired at both ends of the chain (regions marked by the dashed circles in corresponding colors in (a)).

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Mr MORAES, John The University of Sydney, Australia, 1–22 October

Scope of Research

Kinetic and mechanistic analyses are made for better understandings of the chemical and physicochemical reactions occurring in polymerization systems and for better routes to the synthesis of well-defined polymers. By various polymerization techniques, in particular, living polymerizations, new well-defined polymers or polymer assemblies are prepared, and their structure/properties relationships are precisely analyzed. Projects in progress include: (1) Kinetics and mechanisms of living radical polymerization (LRP). (2) Synthesis of new polymeric materials by living polymerizations and their structure/properties studies. (3) Synthesis, properties, and applications of concentrated polymer brushes (CPB).

KEYWORDS

Precision Polymerization
Living Radical Polymerization
Polymer Brush
Hybrid Materials
Biointerface



Selected Publications

Nomura, A.; Okayasu, K.; Ohno, K.; Fukuda, T.; Tsujii, Y., Lubrication Mechanism of Concentrated Polymer Brushes in Solvents: Effect of Solvent Quality and Thereby Swelling State, *Macromolecules*, **44**, 5013-5019 (2011).
Sato, T.; Morinaga, T.; Marukane, S.; Narutomi, T.; Igarashi, T.; Kawano, Y.; Ohno, K.; Fukuda, T.; Tsujii, Y., Novel Solid-State Polymer Electrolyte of Colloidal Crystal Decorated with Ionic-Liquid Polymer Brush, *Adv. Mater.*, **23**, 4868-4872 (2011).
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).

Lubrication of Concentrated Polymer Brushes in Ionic Liquids

Ionic liquids (ILs) have been attracting as new type of lubricants especially at high temperatures and/or under vacuum, by their properties of nonvolatility, noncombustibility and wide solvent-temperature ranges. We have investigated lubrication mechanism of concentrated polymer brushes (CPBs) in solvent (Figure 1), which develops super lubrication property affording ultra-low frictional coefficient μ on the order of 10^{-4} . One of the requirements for establishing the super lubrication of CPBs is good solvent condition, in which the brush layers are sufficiently swollen to their fully-stretched grafted chains. Using the ILs as swelling solvents of CPBs attracts us to the further elucidation of lubrication mechanism and designing practical lubricating surface of CPBs. We have recently observed hydrodynamic lubrication feature in the friction of CPBs in ILs, and their μ values were scaled with the viscosities of pure ILs (Figure 2). These results not only enable us to discuss the details of the effect of solvent viscosity on lubrication of the CPBs, but also demonstrate their ability to act as an excellent lubrication system in combination with ILs as lubricating fluids.

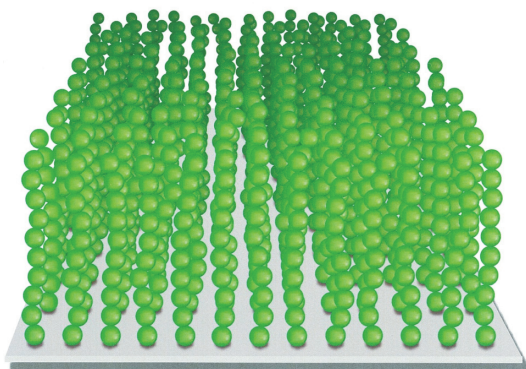


Figure 1. Schematic illustration of concentrated polymer brush.

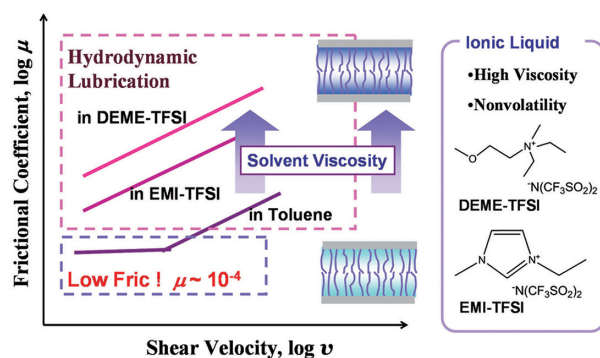


Figure 2. Schematic representation of the friction behavior of concentrated polymer brushes (CPBs) of poly(methyl methacrylate) in ionic liquids (DEME-TFSI and EMI-TFSI) and usual organic solvent (toluene).

Surface-Initiated RAFT Polymerization from Fine Particles

Monodisperse silica particles (SiPs) were surface-modified with a newly designed reversible addition-fragmentation chain transfer (RAFT) agent having a triethoxysilane moiety, 6-(triethoxysilyl)hexyl 2-(((methylthio)carbonothioyl)thio)-2-phenylacetate (EHT) (Figure 3). Surface-initiated RAFT polymerization of styrene was carried out with the EHT-modified SiPs in the presence of a free RAFT agent. The polymerization proceeded in a living manner, producing SiPs coated with well-defined polystyrene of a target molecular weight with a graft density as high as 0.3 chains/nm². Similarly, polymerizations of methyl methacrylate (MMA), *N*-isopropylacrylamide, and *n*-butyl acrylate were conducted, providing SiPs grafted with concentrated (high-density) polymer brushes. In all examined cases, the hybrid particles were highly dispersible in solvents for graft polymers, without causing any aggregations. Owing to exceptionally high uniformity and perfect dispersibility, these hybrid particles formed two- and three-dimensionally ordered arrays at the air-water interface and in suspension, respectively. In addition to the surface-grafting on SiPs, the versatility of this technique was demonstrated by carrying out surface-initiated RAFT polymerization of styrene from iron oxide nanoparticles modified with EHT.

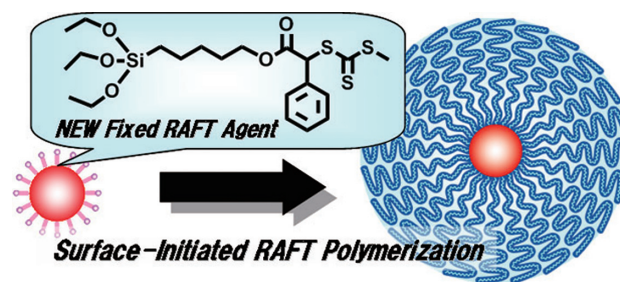


Figure 3. Chemical structure of a newly designed reversible addition-fragmentation chain transfer (RAFT) agent and schematic representation for surface-initiated RAFT polymerization to yield monodisperse silica particles (SiPs) grafted with concentrated (high-density) polymer brushes.

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Prof ASANDEI, Alexandru D. University of Connecticut, U.S.A., 5 October

Scope of Research

Our research focuses on creation of new organic molecules which would become key reagents and materials for future science and technologies. Furthermore, we have been developing new organic and polymeric materials based on our tailor-made molecules. One such topic is the development of new living radical polymerization method utilizing heavier heteroatom compounds as controlling agents. The other topic is the synthesis of cycloparaphenylenes, hoop-shaped π -conjugated molecules, based on new synthetic strategy. We also study various polymer condensed states by both static and dynamic methods to understand the relation of physical properties and structures.

KEYWORDS

Organic Synthesis Polymer Properties
Polymer Synthesis Conjugated π -molecules
Living Radical Polymerization

Selected Publications

Iwamoto, T.; Watanabe, Y.; Sakamoto, Y.; Suzuki, T.; Yamago, S., Selective and Random Syntheses of [*n*]Cycloparaphenylenes (*n* = 8–13) and Size-Dependence of Their Electronic Properties, *J. Am. Chem. Soc.*, **133**, 8354-8361 (2011).
Iwamoto, T.; Watanabe, Y.; Sadahiro, T.; Haino, T.; Yamago, S., Size-Selective Encapsulation of C₆₀ by [10]Cycloparaphenylene. Formation of the Shortest Fullerene-Peapod, *Angew. Chem. Int. Ed.*, **50**, 8342-8344 (2011).
Kayahara, E.; Yamada, H.; Yamago, S., Generation of Carbanions via Stibin-Metal and Bismuthine-Metal Exchange Reaction and Its Applications to Precision Synthesis of ω -End Functionaized Polymers, *Chem. Eur. J.*, **17**, 5272-5280 (2011).
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Yamago, S., Precision Polymer Synthesis by Degenerative Transfer Controlled/Living Radical Polymerization Using Organotellurium, Organostibine, and Organobismuthine Chain Transfer Agents, *Chem. Rev.*, **109**, 5051-5068 (2009).
Tosaka, M., A Route for the Thermodynamic Description of Strain-Induced Crystallization in Sulfur-Cured Natural Rubber, *Macromolecules*, **42**, 6166-6174 (2009).

Formation of the Shortest Fullerene-Peapod

Cycloparaphenylenes (CPPs) are hoop-shaped π -conjugated molecules in which paraphenylene units are linked in a cyclic manner. They represent the simplest structural unit of armchair carbon nanotubes (Figure 1). Based on the analogy to layered carbon networks with curved surfaces, the concave cavity of the CPPs should act as a host for π -conjugated molecules with a convex surface, such as fullerenes. Such a host-guest complex would be a suitable model for elucidating convex-concave π - π interactions. We found that [10]CPP selectively encapsulated C_{60} forming the shortest fullerene-peapod, $[10]CPP \supset C_{60}$, among several CPPs prepared by the method we have developed (Figure 2). This finding opens the possibility of utilizing CPPs as size- and shape-selective host molecules for various guest molecules, such as higher fullerenes, metallofullerenes, and carbon nanotubes. Such complementary host-guest chemistry will be useful for the size- and shape-selective separation of higher fullerenes and carbon nanotubes.

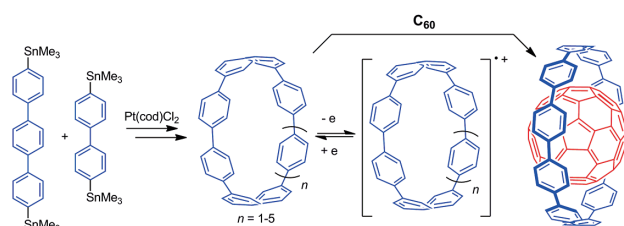


Figure 1. Synthesis and properties of CPPs.

Controlled Copolymerization of (Meth)acrylates and Vinyl Ethers by TERP, SBRP, and BIRP

Synthesis of structurally well-defined macromolecules with controlled molecular weights, molecular weight distributions, functional groups, and monomer sequences by controlled polymerization has been a significant challenge. Such macromolecules would lead to the development of new polymeric materials with improved or novel properties. Random copolymers comprised of (meth)acrylates and vinyl ethers with controlled molecular weights and polydispersities were successfully synthesized by using organotellurium-, organostibine-, and organobismuthine-mediated living radical polymerizations, which are abbreviated as TERP, SBRP, and BIRP, respectively. Highly alternating copolymers were formed for the first time by employing excess amount of vinyl ethers over (meth)acrylates (Figure 2). Several new block copolymers were synthesized by combining the alternating copolymerization and living radical or living cationic polymerization. These methods open new possibilities for providing novel functional polymers in materials science.

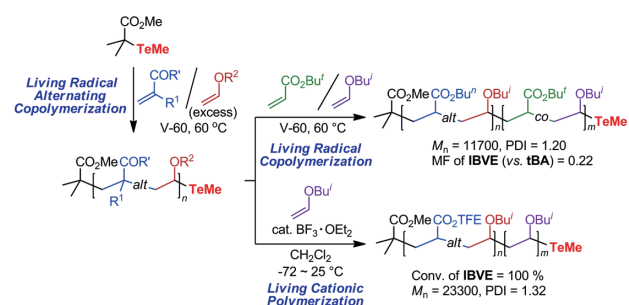
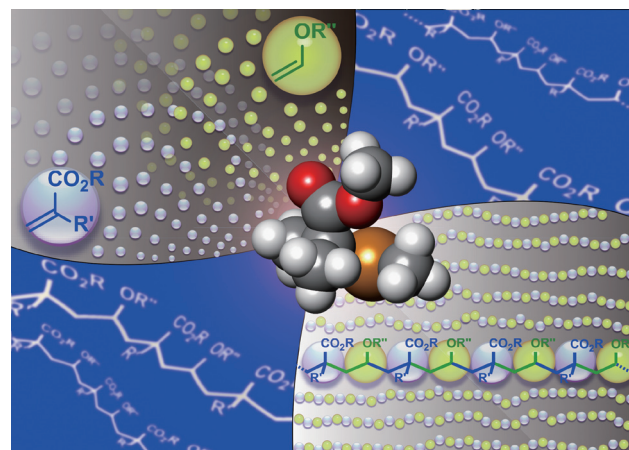
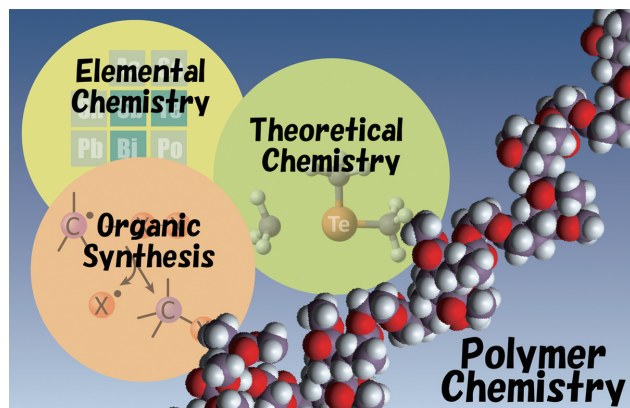


Figure 2. Controlled copolymerization of (meth)acrylates and vinyl ethers by using TERP, SBRP, and BIRP.



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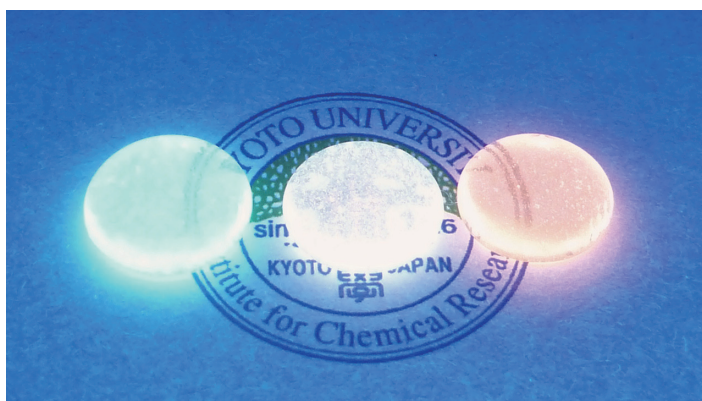
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Scope of Research

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

KEYWORDS

Organic-inorganic Hybrid Materials
Low Melting Glass
Proton Conducting Membrane
Optical Microbiosensor
Amorphous Oxide Phosphor



Selected Publications

- Tokuda, Y.; Oka, T.; Takahashi, M.; Yoko, T., Inhomogeneous Distribution of Na⁺ in Alkali Silicate Glasses, *J. Ceram. Soc. Japan*, **199**, 909-915 (2011).
Tokuda, Y.; Nishioka, S.; Ueda, Y.; Koyanaka, H.; Masai, H.; Takahashi, M.; Yoko, T., Organic-Inorganic Hybrid Titanophosphate Proton Conductive Membranes with Graded Monomer Conversion, *Solid State Ionics*, doi:10.1016/j.ssi.2011.10.028 (2011).
Masai, H.; Takahashi, Y.; Fujiwara, T.; Matsumoto, S.; Yoko, T., High Photoluminescent Property of Low-Melting Sn-Doped Phosphate Glass, *Applied Physics Express*, **3**, [082102-1]-[082102-3] (2010).
Masai, H.; Fujiwara, T.; Matsumoto, S.; Takahashi, Y.; Iwasaki, K.; Tokuda, Y.; Yoko, T., White Light Emission of Mn-Doped SnO-ZnO-P₂O₅ Glass Containing No Rare Earth Cation, *Optics Letters*, **36**, 2868-2870 (2011).

Preparation of Proton Conductive Membranes with Graded Monomer Conversion

Future advances in fuel cell technology are contingent on the development of new materials. One such material is the Nafion membrane (DuPont); it is a proton-conducting membrane and has been employed in polymer electrolyte fuel cells (PEFCs). However, the PEFC faces problems including poor carbon monoxide tolerance and heat rejection in temperatures between 60 and 80°C. In order to overcome these drawbacks, a proton-conducting membrane is required to operate at intermediate temperatures around 100–150°C and should possess good durability and thermal stability.

In this study, we describe a novel technique to prepare a membrane with a graded monomer conversion using ultraviolet light (UV) irradiation during radical photopolymerization. A schematic procedure is shown in Figure 1. High conversion at the surface of the membrane enhanced durability while low conversion at the inner part of the membrane facilitated proton conductivity. This incremental change in the proton conductivity is possible because pKa1 of vinylphosphonic acid (VPA) is 2.74 and pKa2 is 7.34, while pKa of PVPA is around 5–6. Copolymerization of VPA with an additive monomer of hydrophobic nature having a low chain transfer constant leads to an increase in the conversion of the additive polymer.

The proton conductivity of the present membrane was $6.3 \times 10^{-4} \text{ Scm}^{-1}$ at 150°C even under dry conditions. The durability of the membrane VET-ht was much higher than that of polyvinylphosphonic acid, PVPA. The membrane was also thermally stable up to 200°C. These properties contribute to overcome the conventional problems associated with decreases in proton conductivity of polymer electrolytes at intermediate temperatures between 100 and 150°C.

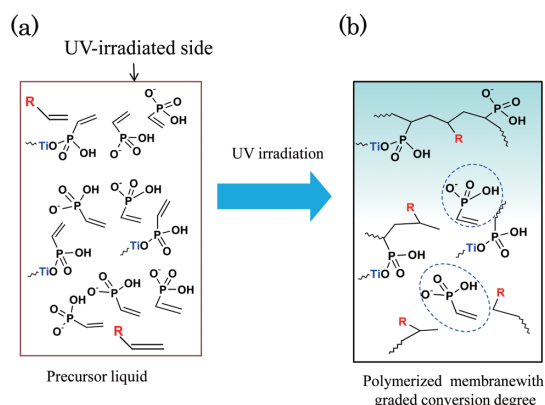


Figure 1. Schematic representation of membrane with graded degrees of polymerization:
(a) titanophosphite precursor.
(b) copolymerized membrane with graded degrees of polymerization.

Fabrication of Rare Earth-free Amorphous Oxide Phosphor

Nowadays, rare earth (RE)-containing materials have been used as white-emitting devices. However, these white-emitting devices consisting of sharp emission bands of RE possess lower color rendering than the conventional broad band emission device. Moreover, since there is uncertainty about the stable supply of RE over the future, it is worthwhile to examine RE-free emitting material.

We have focused on the RE-free phosphors that have been used for white fluorescent lamp. It is expected that white light emission can be attained by RE-free phosphor, for example Sb^{3+} , Mn^{2+} -doped calcium halophosphate. On the other hand, if glass material without the RE cation shows white light emission comparable to the crystalline phosphor, it will be considered a novel emitting material capable of much broader emission and good formability that is quite important in the industrial manufacturing process.

Recently, we have reported the highest quantum efficiency (QE) for amorphous $\text{SnO-ZnO-P}_2\text{O}_5$ low-melting glass. It is notable that the transparent oxide glass containing no RE cation shows high UV-excited emission that is comparable to crystal phosphor such as MgWO_4 ; further, this was the largest efficiency of glass material without RE cation ever reported. The broad emission is brought about by Sn^{2+} , which is the most conventional and harmless ns^2 type center. Our group has also demonstrated white light emission of RE-free Mn-doped $\text{SnO-ZnO-P}_2\text{O}_5$ glass. The transparent glass showed blue ~ white ~ red emission, which depended on the amount of MnO (Figure 2). In particular, some glasses showed white light emission with a high value of quantum efficiency comparable to conventional MgWO_4 crystalline phosphor.

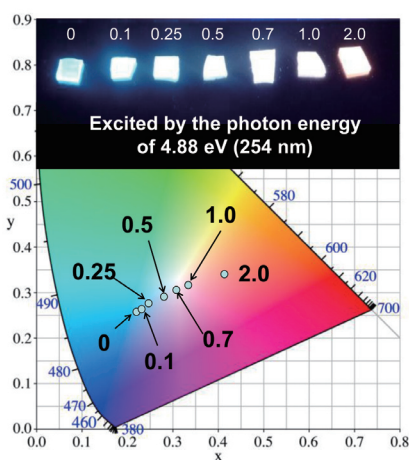


Figure 2. Chromatic coordination mapping of the $x\text{MnO-2.5SnO-57.5 ZnO-40P}_2\text{O}_5$ glasses. Inset shows a photograph of these glasses under exposure to the photon energy of 4.88 eV (254 nm).

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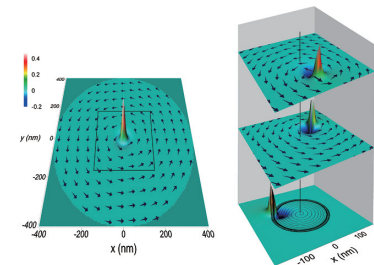
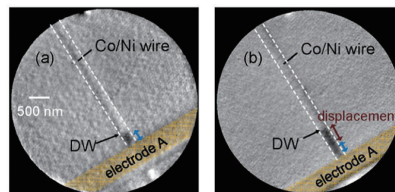
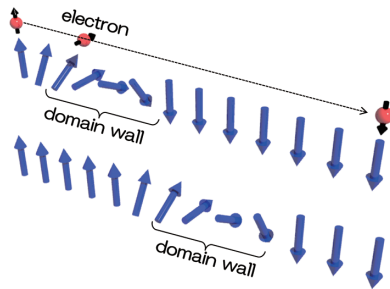
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Scope of Research

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

Yamaguchi, A.; Ono, T.; Nasu, S.; Miyake, K.; Mibu, K.; Shinjo, T., Real-space Observation of Current-Driven Domain Wall Motion in Submicron Magnetic Wires, *Phys. Rev. Lett.*, **92**, [077205-1]-[077205-4] (2004).

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

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

Koyama, T.; Chiba, D.; Ueda, K.; Kondou, K.; Tanigawa, H.; Fukami, S.; Suzuki, T.; Ohshima, N.; Ishiwata, N.; Nakatani, Y.; Kobayashi, K.; Ono, T., Observation of the Intrinsic Pinning of a Magnetic Domain Wall in a Ferromagnetic Nanowire, *Nature Materials*, **10**, 194-197 (2011).

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

Electrical Control of Ferromagnetic Phase Transition

Electrical control of magnetic properties is crucial for device applications in the field of spintronics. Our team has demonstrated the room-temperature electrical control of the ferromagnetic phase transition in cobalt, a representative of the transition-metal ferromagnet family. Solid-state field effect devices, consisting of an ultra-thin cobalt film covered by a dielectric layer and a gate-electrode on top of that, were fabricated (Figure 1). We found that the ferromagnetic state of the film could be turned on and off isothermally and reversed simply by applying gate voltage between the cobalt layer and the gate electrode at room temperature. The shift of the Curie temperature was found to be up to 12 Kelvin by applying gate voltage of ± 10 V. The result is a significant development for future low-power magnetic devices. For example, it could be used for building a “field-effect magnet”; where the magnet can be easily switched-off to become a non-magnet electrically, and for building a non-dissipative magnetic force generator without an electric current. In addition, the demonstrated electric field effect of the two dimensional ferromagnet opens up a new way to explore and control magnetism in relation to the dimensionality.

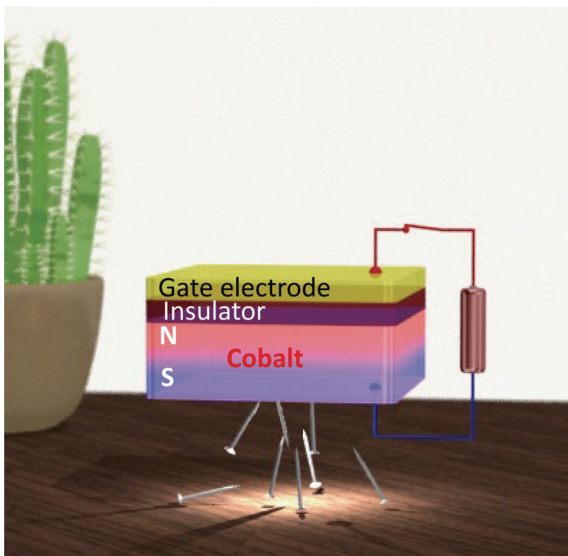


Figure 1. Ferromagnetic phase transition of a metal ferromagnet of Cobalt (Co) was induced by applying a gate voltage (V_G) at room temperature. The device for the transport measurements consists of a metal gate (Au/Cr), an insulator layer (HfO_2), and an ultra-thin Co layer.

Scattered by the Kondo Cloud

The Kondo effect is one of the most fundamental many-body phenomena in condensed matter physics. Conventionally, the Kondo effect is detected through the characteristic temperature dependence of the resistance or the magnetization of the system. Such properties tell us how a local spin interacts with continuum to form a correlated ground state, namely “Kondo cloud”, in lowering the temperature. However, the Kondo effect in an artificial atom or quantum dot (QD) fabricated on the semiconductor surface offers a new attractive stage to address Kondo physics in a way otherwise impossible. We showed that the shot noise at the Kondo QD successfully signals the evolution of the Kondo correlation due to the electron scattering via the Kondo cloud. When the Kondo correlation evolves, the electron scattering that involves several electrons starts to occur. This enhances the shot noise in the Kondo QD more than that in the noninteracting case. Such an experiment can be viewed as “collision experiments” on a chip and will shed new light on Kondo physics.

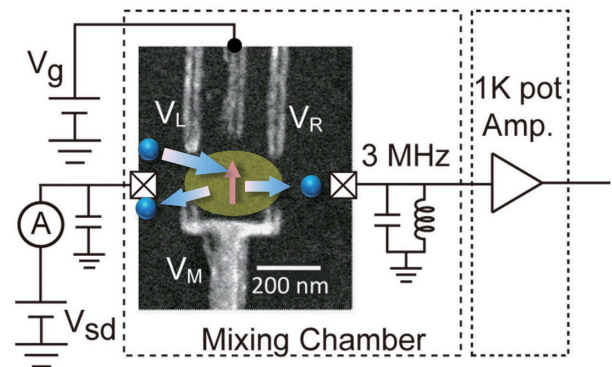


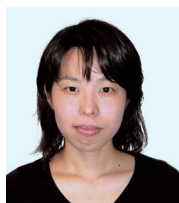
Figure 2. The scanning electron microscope image of the artificial atom (yellow) with a measurement schematic. The single spin inside the atom (indicated by the arrow) causes the Kondo effect. We measure the electron scattering by the Kondo state.

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MURAYAMA, Tomo (UG)
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Visitor

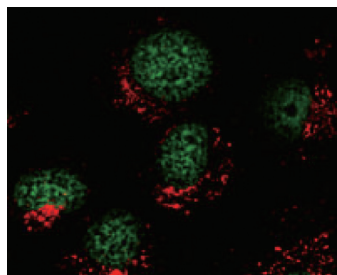
Prof DIBO, Gabor Institute of Chemistry, Eotvos Loránd University, Hungary, 12 December

Scope of Research

The ultimate goal of our research is the regulation of cellular functions by designed peptides and proteins. Current research subjects include (1) development of novel intracellular delivery systems aiming at elucidation and control of cellular functions using designed membrane permeable peptide vectors, (2) elucidation of the DNA binding and recognition modes of C2H2-type zinc finger proteins and design of artificial transcription factors with various DNA binding specificities, and (3) design of stimulation-responsive artificial peptides and proteins.

KEYWORDS

Membrane-Permeable Peptides
Intracellular Delivery
Peptide Design
Zinc Finger Protein



Selected Publications

- Imanishi, M.; Nakamura, A.; Doi, M.; Futaki, S.; Okamura, H., Control of Circadian Phase by an Artificial Zinc Finger Transcription Regulator, *Angew. Chem. Int. Ed.*, **50**, 9396-9399 (2011).
- Imanishi, M.; Nakaya, T.; Morisaki, T.; Noshiro, D.; Futaki, S.; Sugiura, Y., Metal-Stimulated Transcriptional Regulation by an Artificial Zinc Finger Protein, *ChemBioChem*, **11**, 1653-1655 (2010).
- Noshiro, D.; Asami, K.; Futaki, S., Metal-Assisted Channel Stabilization: Disposition of a Single Histidine on the N-terminus of Alamethicin Yielded Channels with Extraordinarily Long Lifetimes, *Biophys. J.*, **98**, 1801-1808 (2010).
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- Inomata, K.; Ohno, A.; Tochio, H.; Isogai, S.; Tenno, T.; Nakase, I.; Takeuchi, T.; Futaki, S.; Ito, Y.; Hiroaki, H.; Shirakawa, M., High-Resolution Multi-Dimensional NMR Spectroscopy of Proteins in Human Cells, *Nature*, **458**, 106-110 (2009).
- Nakase, I.; Hirose, H.; Tanaka, G.; Tadokoro, A.; Kobayashi, S.; Takeuchi, T.; Futaki, S., Cell Surface Accumulation of Flock House Virus-derived Peptide Leads to Efficient Internalization via Macropinocytosis, *Mol. Ther.*, **17**, 1868-1876 (2009).

In Vivo Tumor Accumulation of Arginine-rich Cell-penetrating Peptides and Anticancer Drug Delivery

In this study, we investigated the biodistribution of arginine-rich cell-penetrating peptides (CPPs) in tumor-xenografted nude mice using *in vivo* imaging after the intravenous injection of the fluorescently labeled CPPs. There have been several reports about the *in vivo* distribution of arginine-rich CPPs and their conjugates that often suggest their tendencies to accumulate in some organs. However, few reports have been published that studied the biodistribution of CPPs in tumor-xenografted mice.

Using typical arginine-rich CPPs, this study determined that there is a considerable difference among these peptides regarding their tendencies of tumor accumulation. Tat, Penetratin and octaarginine (R8) showed almost a similar degree of accumulation in the kidney, liver and lung, however, R8 showed a higher accumulation in the tumor xenografts. A comparison of the tendency for tumor accumulation of the oligoarginines composed of different numbers of arginines (R2, R8, R12, and R16) revealed that the R8 peptide showed the highest accumulation in a tumor. A further increase in tumor accumulation was observed by the D-substitution of the amino acids of R8 peptide (r8).

To exemplify the applicability of the r8 peptide for cancer therapy, the conjugate of doxorubicin with r8 was prepared. The r8-doxorubicin conjugate (4 mg doxorubicin/kg) effectively suppressed the tumor proliferation without a decrease in the mouse weight after intravenous injection of the conjugate. A higher dose of doxorubicin (6 mg/kg) was necessary to obtain the same extent of tumor growth suppression effect without conjugation to r8, but this was accompanied by a significant weight loss of the mice. These results suggested the potential of r8 as a prototype of tumor-targeting vectors.

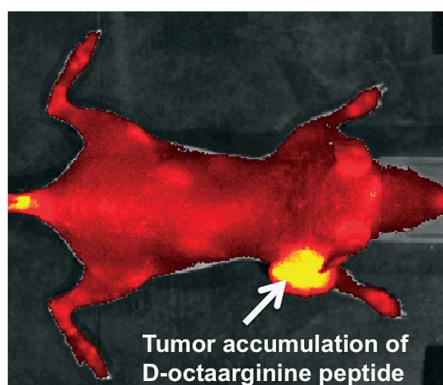


Figure 1. Tumor accumulation of fluorescently labeled r8 peptide intravenously administered into tumor-bearing mouse.

Control of Circadian Phase by an Artificial Zinc Finger Transcription Regulator

Circadian time originates from clock genes interlocked in transcription/translation feedback loops. In spite of the increase in fundamental knowledge of the circadian molecular machinery in the past decade, practical applications have been so far lacking, and no attempts have been performed in the adjustment of circadian time via a direct action on the core-clock components. Recently, C2H2-type zinc-finger-based artificial DNA binding proteins have seen tremendous development, and can be used to specifically and efficiently manipulate the expression of a target gene.

Here we designed a C2H2-type zinc-finger-based artificial DNA binding protein, ZF(dGRE), that can specifically recognize the glucocorticoid responsive element (GRE) in the regulatory region of the *Period1* gene. A chromatin immunoprecipitation (ChIP) assay indicated that the DNA binding activity and sequence specificity of ZF(dGRE) are functionally preserved even when its DNA target site is chromosomally structured within the cells. To control the time-specificity of our zinc-finger construct, we added the ligand-controllable destabilizing domain and a transcriptional activation domain to ZF(dGRE). The ligand-inducible accumulation of this artificial transcription factor in the nucleus led to the consolidation of circadian rhythms and to circadian phase resetting (Figure 2). To our knowledge, this is the first report of an artificially designed protein that can externally control cellular clock at the genomic level. In addition, our results suggest that *mPeriod1* is a state variable in the generation of circadian rhythms. This artificial transcription factor, which directly controls the clock machinery, potentially opens the way towards novel and effective chronotherapy by tuning circadian time.

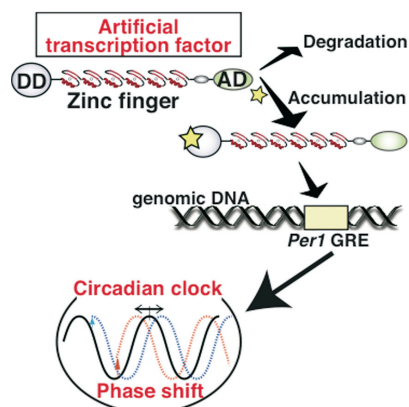


Figure 2. Induction of circadian phase shifts by an artificial transcription factor specifically targeting a glucocorticoid response element of the *mPeriod1* gene.

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Scope of Research

Our research interests focus on the molecular design and synthesis of specific inhibitors of physiologically important enzymes (biocatalysts) for use as chemical probes to understand the reaction mechanisms, three-dimensional structures and physiological roles of the enzymes. The finely designed inhibitors are further elaborated to develop pharmaceuticals and agrochemicals. Our research includes: Design, synthesis and applications of transition-state analogue and mechanism-based inhibitors of the key enzymes in glutathione homeostasis, asparagine synthetase, and the development of intermediate analogue inhibitors of acyl-activating enzyme superfamily that plays pivotal roles in plant hormone and secondary metabolite biosynthesis.

KEYWORDS

Enzyme Reaction Mechanisms
Transition-State Analogue Inhibitors
Glutathione Homeostasis
Bioactivity Substance
Plant Secondary Metabolite Biosynthesis



Selected Publications

- Joyce-Brady, M.; Hiratake, J., Inhibiting Glutathione Metabolism in Lung Lining Fluid as a Strategy to Augment Antioxidant Defense, *Current Enzyme Inhibition*, **7**, 71-77 (2011).
- Koeduka, T.; Watanabe, B.; Suzuki, S.; Hiratake, J.; Mano, J.; Yazaki, K., Characterization of Raspberry Ketone/Zingerone Synthase, Catalyzing the Alpha, Beta-Hydrogenation of Phenylbutenones in Raspberry Fruits, *Biochem. Biophys. Res. Commun.*, **412**, 104-108 (2011).
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- Han, L.; Hiratake, J.; Kamiyama, A.; Sakata, K., Design, Synthesis and Evaluation of γ -Phosphono Diester Analogues of Glutamate as Highly Potent Inhibitors and Active Site Probes of γ -Glutamyl Transpeptidase, *Biochemistry*, **46**, 1432-1447 (2007).

Design, Synthesis and Applications of Specific Inhibitors of γ -Glutamyl Transpeptidase for Modulating Cellular Redox Status

Glutathione (GSH, γ -Glu-Cys-Gly) is an ubiquitous tripeptide containing Cys found in many organisms. It plays central roles in the redox status of cells not only by detoxification of reactive oxygen species, but also by regulating the transcription of specific genes such as phase II antioxidant enzymes. We are interested in regulating the cellular GSH level by controlling the activities of its biosynthetic enzyme, γ -glutamylcysteine synthetase (GCS), and its metabolic enzyme, γ -glutamyl transpeptidase (GGT), by using specific inhibitors (Figure 1). GGT is a key enzyme in supplying the cells with Cys by cleaving the γ -glutamyl bond of extracellular GSH, as well as in degrading GSH conjugates for detoxification. We developed a series of phosphonate-based inactivators of GGT and found that an inhibitor was highly efficient for human GGT. Interestingly, this inhibitor significantly increased the biosynthesis of type I collagen and elastin of human skin fibroblasts and can be used, for example, as a novel antiaging cosmetic ingredient. The study on its mode of action and its application as a novel “cosmeceutical” are in progress.

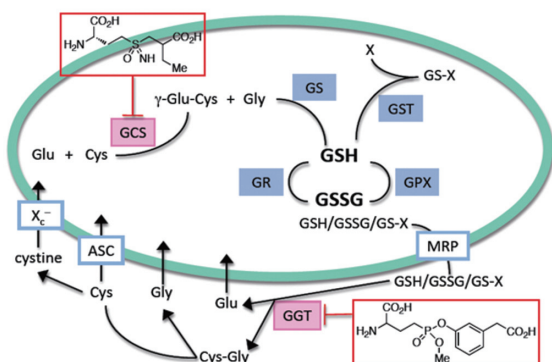


Figure 1. Biosynthesis, reaction, and metabolism of glutathione (GSH) in cell. The specific inhibitors of GCS and GGT are shown in red squares.

Inhibitors Targeting Human Asparagine Synthetase for Cancer Chemotherapy

Human asparagine synthetase (hAS) catalyzes the ATP-dependent synthesis of Asn from Asp using Gln as an ammonia source. The inhibition of hAS is highly important in enhancing and broadening the efficacy of asparaginase chemotherapy of leukemia and cancer. We previously developed the first nano molar *in vitro* hAS inhibitor **1** ($K_i^* = 24$ nM) and succeeded in suppression of proliferation of asparaginase-resistant cancer cell line, but at higher concentrations (100–1000 μ M). The bioavailability of **1**

was increased by removing a carboxy group to eliminate net negative charge. Surprisingly, the new compound **2** inhibited hAS even stronger ($K_i^* = 7.6$ nM) than the original **1** and not only suppressed cell proliferation in a dose-dependent manner, but also induced cell death irrespective of the presence of asparaginase. This result suggests that hAS in itself is a novel target without the aid of asparaginase, which might open a new paradigm for anti-cancer chemotherapy.

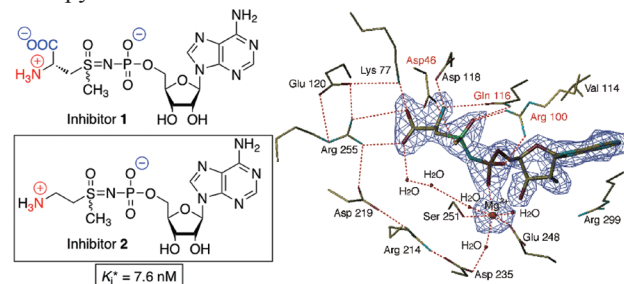


Figure 2. (Left) The structure of the original inhibitor **1** and newly synthesized inhibitor **2**. (Right) X-Ray crystal structure of *E. coli* AS in complex with **1**.

Specific Inhibitors of Acyl-activating Enzymes for “Chemical Knockout”

Acyl-activating enzymes constitute a large enzyme superfamily that contains a number of such important enzymes as for fatty acid β -oxidation and biosynthesis of plant secondary metabolites. In light of their common mechanistic features involving acyl-adenylate intermediate, we designed and synthesized *N*-acyl adenosyl sulfamides as intermediate-analogue inhibitors to probe the physiological impact of a key enzyme 4-coumaric acid:CoA ligase (4CL) on phenylpropanoid biosynthesis. The synthetic compounds inhibited 4CL *in vitro*, and the substituents on benzene ring significantly affected their potency. Administration of the inhibitors to *Arabidopsis* caused decrease of the phenylpropanoids contents. This result implied that the inhibitors were up-taken by plants and inhibited 4CL *in vivo*. The inhibitors are promising tools for chemical biology of plants for controlling plant secondary metabolites including the phenylpropene volatiles and lignin biosynthesis.



Figure 3. The outline of phenylpropanoid biosynthesis and the structure of intermediate analogue inhibitors.

Division of Biochemistry – Molecular Biology –

http://molbio.kuicr.kyoto-u.ac.jp/mb/index_e.html



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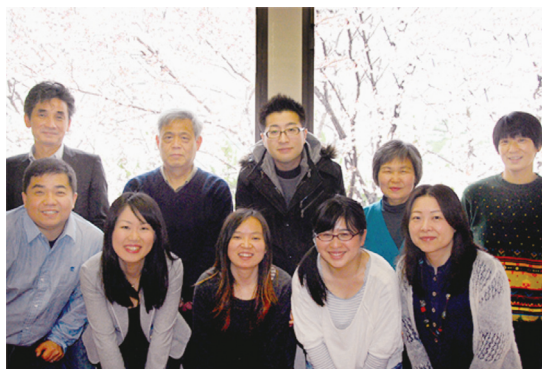
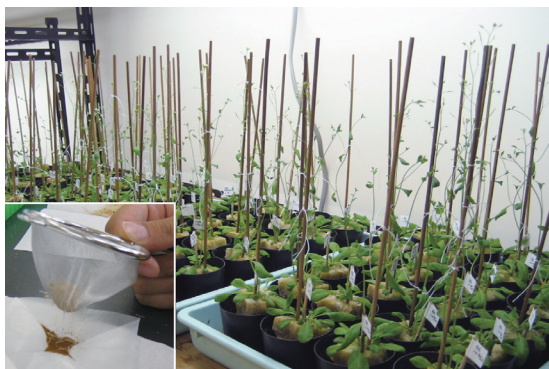
Ms LUO, Yu College of Life Science, Peking University, China, P.R., 6 October 2010–5 October 2011
Ms WEI, Jia College of Life Science, Peking University, China, P.R., 6 October 2010–5 October 2011

Scope of Research

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

KEYWORDS

Morphogenesis
Signal Transduction
Phospholipid
COP9 Signalosome
Cytokinin



Selected Publications

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Mechanism of Spliceosomal Protein in Its Requirement for Pollen Development

In flowering plants, the male gametophyte plays a vital role in plant fertility through the generation and delivery of the sperm cells to the embryo sac for double fertilization. During male gametogenesis, diploid pollen mother cells undergo meiotic division to produce tetrads of haploid microspores. The microspores are then released from tetrads and undergo an asymmetric cell division to produce bicellular pollen grains that contain a generative cell and a much larger vegetative cell. The smaller generative cells continue through another round of mitosis to produce twin sperm cells, composing the tricellular pollen grains.

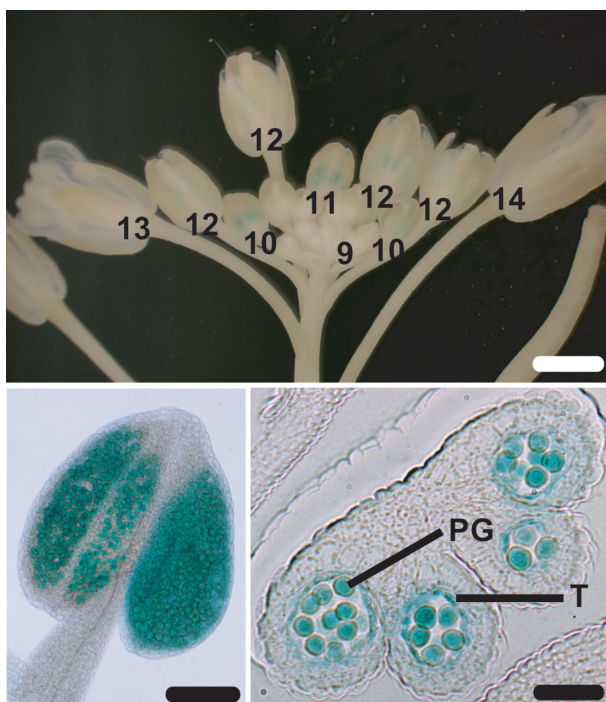


Figure 1. GUS staining of *AtSAP130a* pro-GUS plants revealed strong promoter activity in the theca (below left), specifically at stages 10 to 12 of flower development (above). Stages are indicated with numbers. Transverse sections of anther show strong GUS signals in the tapetum and pollen grains (below right). T, tapetum; PG, pollen grain. Bars = 1 mm (above), 100 μ m (below left), or 50 μ m (below right).

We found that the *Arabidopsis* spliceosomal protein, SPLICEOSOME-ASSOCIATED PROTEIN 130 (*AtSAP130*), was required for proper pollen development. Although *SAP130* is essential for mRNA splicing and the formation of the pre-spliceosome, its detailed function remains unclear. *AtSAP130* is encoded by two genes, *AtSAP130a* and *AtSAP130b*. Activities of the promoters of these genes overlapped at specific stages of anther and pollen development (Figure 1). Plants with reduced expression of the *AtSAP130* genes, induced by RNA interference (*AtSAP130* RNAi), showed developmental defects in the pollen during the transition from microspore to bicellular stages of male gametogenesis (Figure 2).

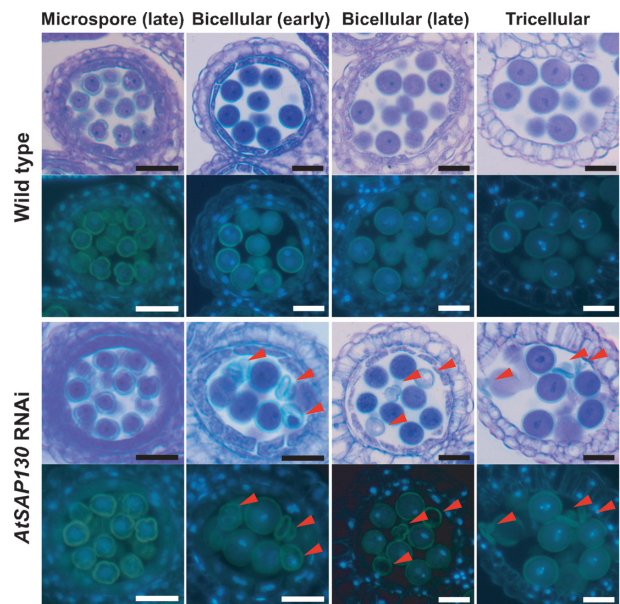


Figure 2. Histological analyses of pollen development in wild type and *AtSAP130* RNAi plants. Upper panels show the transverse light-field images of the anther locules stained with toluidine blue, while lower panels show the corresponding UV-field images stained with DAPI. Red arrowheads indicate deformed non-viable pollen grains detected at the bicellular stage and later. Bars = 25 μ m.

In attempt to identify genes responsible for the pollen deficiency in the *AtSAP130* RNAi plants, we analyzed the expression of key genes in anther and pollen development. *QRT1* and *QRT3*, which have been shown to be required for microspore separation, preferentially accumulated less mRNA in *AtSAP130* RNAi plants (Figure 3). Although the two *QRT* genes might not be the direct cause for the pollen defect we observed in the *AtSAP130* RNAi plants, this could be due to the partial but not complete knock-down of the *QRT* genes. Taken together, these results suggested that *AtSAP130a* and *AtSAP130b* play an indispensable role in specific spatiotemporal events during pollen development.

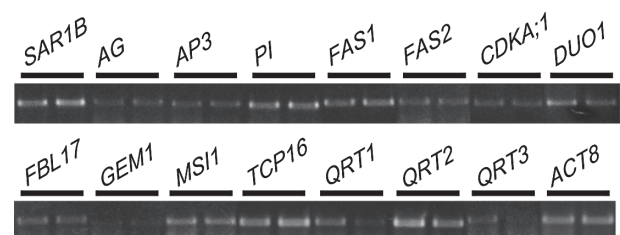


Figure 3. Expression analysis of key genes involved in pollen development. Semi-quantitative RT-PCR was performed on 14 representative genes expressed in the anther and post-tetrad stage of pollen development. *SAR1B* was also analyzed as a putative target, based on a former report in yeast. *ACT8* was used as a control.

Previously, we revealed that *SAP130* binds to COP9 signalosome (CSN) in human and *Arabidopsis*. CSN regulates signal transduction through its control on proteolysis. We are exploring the venue where the interaction between CSN and *SAP130* would bridge regulations of mRNA maturation and proteolysis.

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Prof KIM, Sunghoon Seoul National University, Korea, R., 5 October
Prof LEE, Kyeong Dongguk University, Korea, R, 28 November

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 by using chemistry. Our laboratory has been discovering or designing unique organic molecules that modulate fundamental processes in human cells. Our mission is to create new world of bioactive synthetic molecules: their new way to use, their new shapes, and their new sizes. We hope to open new avenues for small-molecule applications in a range of fields, including future concepts in drug discovery and use of small molecules for cell therapy.

KEYWORDS

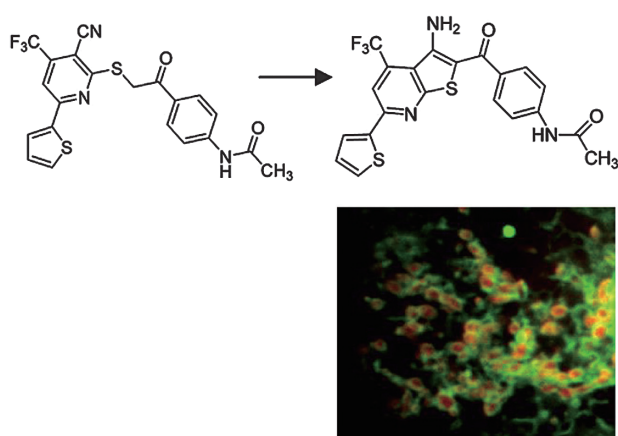
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

Selected Publications

- Kawazoe, Y.; Shimogawa, H.; Sato, A.; Uesugi, M., Mitochondrial Surface-specific Fluorescent Probe Activated by Bioconversion, *Angew. Chem. Int. Ed.*, **50(24)**, 5478-5481 (2011).
- Sumiya, E.; Shimogawa, H.; Sasaki, H.; Tsutsumi, M.; Yoshita, K.; Ojika, M.; Suenaga, K.; Uesugi, M., Cell-morphology Profiling of a Natural Product Library Identifies Bisbromoamide and Miuraenamamide A as Actin-filament Stabilizers, *ACS Chem. Biol.*, **6(5)**, 425-431 (2011).
- Shirakawa, T.; Kawazoe, Y.; Tsujikawa, T.; Jung, D.; Sato, S.; Uesugi, M., Deactivation of STAT6 through Serine 707 Phosphorylation by JNK, *J. Biol. Chem.*, **286**, 4003-4010 (2011).
- Sato, S.; Murata, A.; Orihara, T.; Shirakawa, T.; Suenaga, K.; Kigoshi, H.; Uesugi, M., Marine Natural Product Aurilide Activates the OPA1-mediated Apoptosis by Binding to Prohibitin, *Chem. Biol.*, **18 (1)**, 131-139 (2011).
- Kamisuki, S.; Shirakawa, T.; Kugimiya, A.; Abu-Elheiga, L.; Choo, H. Y.; Yamada, K.; Shimogawa, H.; Wakil, S. J.; Uesugi, M., Synthesis and Evaluation of Diarylthiazole Derivatives that Inhibit Activation of Sterol Regulatory Element-binding Proteins, *J. Med. Chem.*, **54(13)**, 4923-4927(2011).
- Murata, A.; Sato, S.; Kawazoe, Y.; Uesugi, M., Small-molecule Fluorescent Probes for Specific RNA Targets, *Chem. Comm.*, **47**, 4712-4714 (2011).

A Mitochondrial Surface-specific Fluorescent Probe Activated by Bioconversion

We carried out cell-based image screening of 12,000 small molecules enriched in aromatic groups and identified thirty-one that had potential as fluorescent probes for living cells. One of the candidates appeared to selectively stain mitochondrial surfaces. Results of spectroscopic analyses and chemical synthesis indicated that the molecule underwent metabolic cyclization to be fluorescent inside cells. To our knowledge, this molecule represents the first fluorescent probe specific for mitochondrial surfaces.



Cell-morphology Profiling of a Natural Product Library

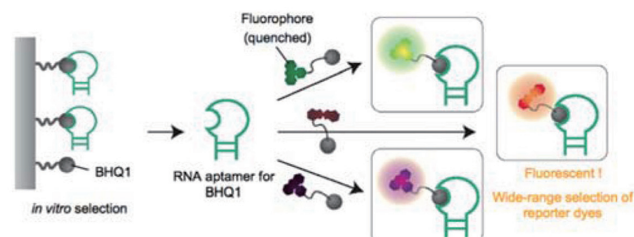
Natural products provide a rich source of biological tools, but elucidating their molecular targets remains challenging. We carried out a cell morphological profiling of a natural product library, which permitted the identification of bisbromoamide and miuraenamides A as actin filament stabilizers. Automated high-content image analysis showed that these two structurally distinct marine natural products induce morphological changes in HeLa cells similar to those induced by known actin-stabilizing compounds. Bisbromoamide and miuraenamide A stabilized actin filaments *in vitro*, and fluorescein-conjugated bisbromoamide localized specifically to actin filaments in cells. Cell morphological profiling was also used to identify actin-stabilizing or -destabilizing natural products from marine sponge extracts, leading to the isolation of pectenotoxin-2 and lyngbyabellin C. Overall, the results demonstrate that high-content imaging of nuclei and cell shapes offers a sensitive and convenient method for detecting and isolating molecules that target actin.

Discovery of FGH10019

In 2009, our group reported the discovery and synthesis of “fatostatin,” a small molecule that inhibits activation of sterol regulatory element-binding protein (SREBP). Fatostatin blocks biosynthesis and accumulation of fat in obese mice. We newly synthesized and evaluated a series of fatostatin derivatives. Our structure-activity relationships led to the identification of FGH10019 as the most potent drug-like molecule among the analogues tested. FGH10019 has high aqueous solubility and membrane permeability and may serve as a seed molecule for further development.

Small-molecule Fluorescent Probes for Specific RNA Targets

A method was developed that uses small molecules as fluorescent probes to detect specific mRNAs. In this approach, the fluorescence of fluorophore-quencher conjugates is restored by the binding of an mRNA aptamer tag to the quencher segment of the molecules. The method allows real-time detection of mRNA transcripts *in vitro*.



Division of Environmental Chemistry – Molecular Materials Chemistry –

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Scope of Research

Our research target is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. For the purpose, we have carried out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, detailed analyses of structures and dynamics are performed mainly by sophisticated solid-state NMR spectroscopy in order to obtain structure-dynamics-property relationships.

KEYWORDS

Solid-State NMR
Amorphous Materials
Organic Light-Emitting Diodes

Living Radical Polymerization
Quantum Chemical Calculation

Selected Publications

Fukushima, T.; Kimura, H.; Shimahara, Y.; Kaji, H., Solid-State Nuclear Magnetic Resonance Analysis of Phase Separation Behavior of Regioregular Poly(3-hexylthiophene) and [6,6]-Phenyl-C₆₁-Butyric Acid Methyl Ester in Bulk Heterojunction Organic Solar Cells, *Appl. Phys. Lett.*, **99**, [223301-1]-[223301-3] (2011). (Selected for the November 2011 Issue of APL: Organic Electronics and Photonics.)

Goto, A.; Suzuki, T.; Ohfuji, H.; Tanishima, M.; Fukuda, T.; Tsujii, Y.; Kaji, H., Reversible Complexation Mediated Living Radical Polymerization (RCMP) Using Organic Catalysts, *Macromolecules*, **44**, 8709-8715 (2011).

Tokudome, Y.; Fukushima, T.; Goto, A.; Kaji, H., Enhanced Hole Injection in Organic Light-Emitting Diodes by Optimized Synthesis of Self-Assembled Monolayer, *Org. Electron.*, **12**, 1600-1605 (2011).

Kaji, H.; Hayashi, H.; Yamada, T.; Fukuchi, M.; Fujimura, S.; Ueda, M.; Kang, S.; Umeyama, T.; Matano, Y.; Imahori, H., Local Stoichiometry in Amorphous Supramolecular Composites Analyzed by Solid-State ¹³C Nuclear Magnetic Resonance, *Appl. Phys. Lett.*, **98**, [113301-1]-[113301-3] (2011). (Selected for the March 2011 Issue of APL: Organic Electronics and Photonics. Selected for the March 28, 2011 Issue of Virtual Journal of Nanoscale Science & Technology.)

Yamada, T.; Suzuki, F.; Goto, A.; Sato, T.; Tanaka, K.; Kaji, H., Revealing Bipolar Charge-Transport Property of 4,4'-N,N'-dicarbazolylbiphenyl (CBP) by Quantum Chemical Calculations, *Org. Electron.*, **12**, 169-178 (2011).

Solid-State NMR Analysis of Donor-Acceptor Structure in Bulk Heterojunction Organic Solar Cells

The origin of the improvement in power conversion efficiency (PCE) by the thermal annealing of bulk heterojunction organic solar cells, based on regioregular poly(3-hexylthiophene-2,5-diyl) (rrP3HT) and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM), is analyzed by solid-state nuclear magnetic resonance (NMR). ¹H spin-lattice relaxation experiments of solid-state NMR clearly reveal that the phase-separated heterojunction structure develops on the order of several tens of nanometers in rrP3HT/PCBM blend films with thermal annealing at 150°C. The development of the phase-separated structure explains the increase in the PCE for the solar cell system from 0.7% to nearly 3% through the thermal annealing.

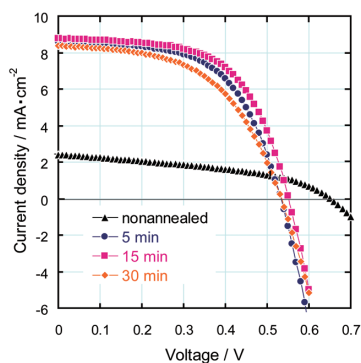


Figure 1. J–V curves obtained from rrP3HT/PCBM bulk heterojunction OSCs under AM 1.5 illumination at an irradiation intensity of 100 mW/cm². The annealing temperature is 150°C. The annealing times are shown in the figure.

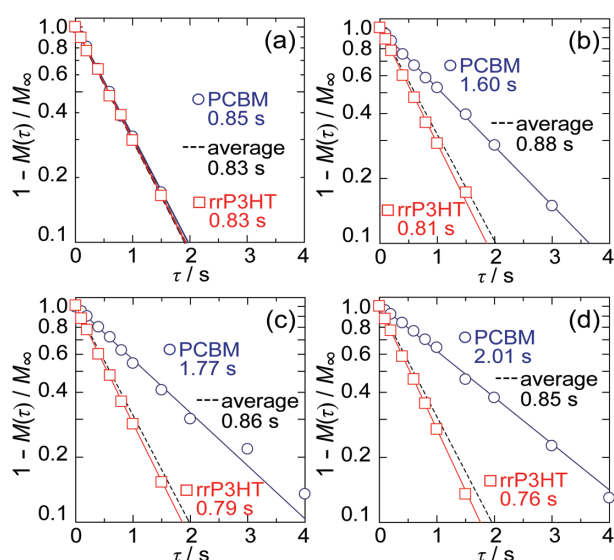


Figure 2. ¹H spin-lattice relaxation curves of rrP3HT (□) and PCBM (○) components in rrP3HT/PCBM blends; (a) as-cast, annealed at 150°C for (b) 5 min, (c) 15 min, and (d) 30 min. The average relaxation curves for rrP3HT and PCBM are also shown as broken lines.

Living Polymerization of Styrene with Gallium Catalyst towards Control of Molecular Weight and Tacticity

A living polymerization using iodine as a capping agent and a gallium compound (GaI₃) as a catalyst was studied. The polymerization of styrene yielded well-defined polymers with predetermined molecular weights and narrow molecular weight distribution (PDI=1.2–1.5) up to about 70% monomer conversion. Interestingly, the catalyst did not only achieve small PDI but also changed tacticity (stereoregularity) from that of a free radical propagating species. This indicates the (co)existence of another type of propagating species and a potential for dual control of PDI and tacticity with a single catalyst.

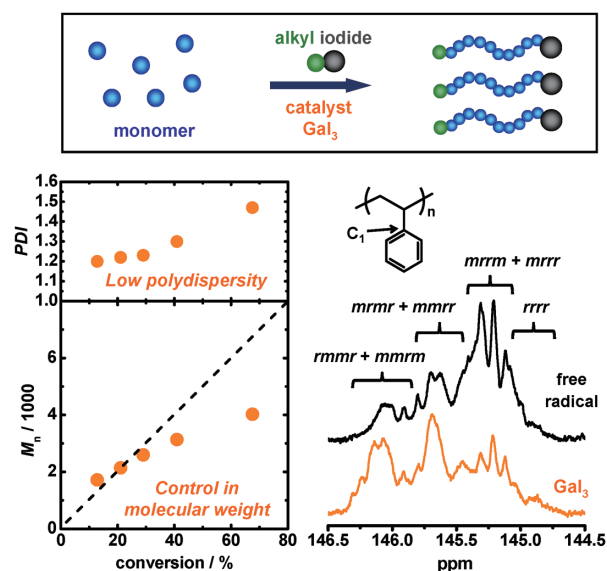


Figure 3. Schematic illustration of gallium-catalyzed polymerization, plots of M_n (molecular weight) and PDI vs monomer conversion, and ¹³C NMR spectra for phenyl C1 carbon taken by 800 MHz NMR (200 MHz ¹³C NMR) spectrometer.

Division of Environmental Chemistry – Hydrospheric Environment Analytical Chemistry –

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Scope of Research

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

KEYWORDS

Analytical Chemistry
Marine Chemistry
Trace Elements
Stable Isotopes
Metal Ion Recognition



Selected Publications

- Firdaus, M. L.; Minami, T.; Norisuye, K.; Sohrin, Y., Strong Elemental Fractionation of Zr-Hf and Nb-Ta across the Pacific Ocean, *Nature Geoscience*, **4**, 227-230 (2011).
- Li, Y. -H.; Sohrin, Y.; Takamatsu, T., Lake Biwa and the Ocean: Geochemical Similarity and Difference, *Limnology*, **12**, 89-101 (2011).
- Sohrin, Y.; Bruland, K. W., Global Status of Trace Elements in the Ocean, *TrAC Trends in Analytical Chemistry*, **30**, 1291-1307 (2011).
- Cid, A. P.; Urushihara, S.; Minami, T.; Norisuye, K.; Sohrin, Y., Stoichiometry among Bioactive Trace Metals in Seawater on the Bering Sea Shelf, *Journal of Oceanography*, **67**, 747-764 (2011).

Strong Elemental Fractionation of Zr–Hf and Nb–Ta across the Pacific Ocean

Understanding the circulation of water masses in the world's oceans is critical to our knowledge of the Earth's climate system. Trace elements and their isotopes have been explored as tracers for the movement of water masses. One type of candidate elements is the high-field-strength elements zirconium (Zr), hafnium (Hf), niobium (Nb) and tantalum (Ta). Here we measure the distributions of dissolved Zr, Hf, Nb and Ta along two meridional sections in the Pacific Ocean that extend from 65°S to 10°N and from 10°S to 50°N. We find that all four elements tend to be depleted in surface water. In the deep oceans, their concentrations rise along our transects from the Southern Ocean to the North Pacific Ocean, and show strong correlations with the concentration of silicate. These results indicate that terrigenous sources are important to the budget of Zr, Hf, Nb and Ta in seawater, compared with hydrothermal input. Unexpectedly, the weight ratios for Zr/Hf fall between 45 and 350 and those for Nb/Ta between 14 and 85 in Pacific seawater, higher than the ratios observed in fresh water, in the silicate Earth or in chondritic meteorites. We conclude that the fractionation of Zr/Hf and Nb/Ta ratios will be useful for tracing water masses in the ocean.

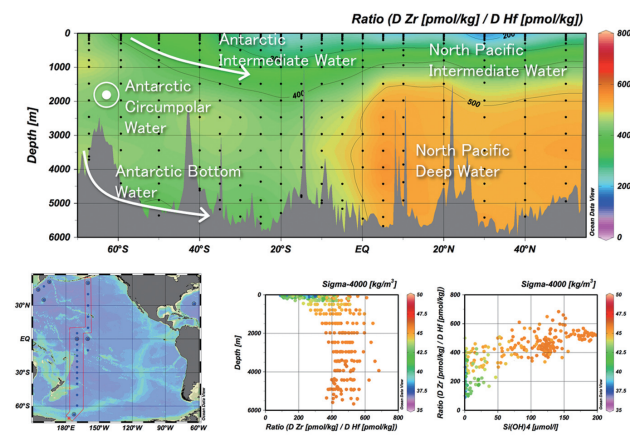


Figure 1. Meridional sectional distribution of DZr/DHf and water masses in the Pacific Ocean.

Stoichiometry among Bioactive Trace Metals in Seawater on the Bering Sea Shelf

The distribution of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in seawater was investigated on the Bering Sea shelf (56–64°N, 165–169°W) in September 2000. The unfiltered and filtered seawater samples were used for determination of total dissolvable (TD) and dissolved (D) metals (M), respectively. The TDM concentrations were generally higher than in the Pacific Ocean. TDCd was highest in deep water of the outer shelf domain and dominated by dissolved species. The other TDM were highest at stations close to the Yukon River delta and had higher fractions of labile particulate (LP) species that were obtained as the difference between TDM and DM. DAI, DNi, and DCu were characterized by input from the Yukon River. DMn and DCo showed maximums on the bottom of the coastal domain, suggesting influence of sedimentary Mn reduction. The correlations of DZn, DCd, and macronutrients indicated their distributions were largely controlled through uptake by microorganisms and remineralization from settling particles. All these three processes (river input, sedimentary reduction, and biogeochemical cycle) had influence on the distribution of DFe. DPb was fairly uniformly distributed in the study area. The stoichiometry of DMs in the Bering Sea shelf showed enrichment of Co and Pb and depletion of Ni, Cu, Zn, and Cd compared to that in the North Pacific. The LPM/LPAI ratio revealed significant enrichment of the other eight metals against the crustal abundance, suggesting importance of formation of Fe-Mn oxides and adsorption of trace metals on the oxides.



Figure 2. Observation in the Bering Sea during the R/V Mirai MR00-K06 cruise in September 2000.

Division of Environmental Chemistry – Solution and Interface Chemistry –

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Scope of Research

We investigate the chemical phenomenon in two kinds of condensed phases. (1) To understand the chemical structure, property and reactions in a two-dimensional molecular aggregated ultrathin film, the keywords of molecular interactions and orientation are additionally employed, and the fluctuated molecular aggregates are investigated by originally developed spectroscopic and theoretical techniques. (2) The structure, dynamics, and reaction of solutions with nano-scale inhomogeneity and/or with fine tunability are investigated by computer simulation, and statistical-mechanical theory of solutions, and NMR spectroscopy.

KEYWORDS

Infrared and Raman Spectroscopy	Free Energy
Surface and Interface Chemistry	Solvation
Spectral Analysis	Solution Theory



Selected Publications

Kasuya, A.; Itoh, Y.; Okada, T.; Osawa, M.; Takahashi, Y.; Kazuma, E.; Tatsuma, T.; Hasegawa, T., Anisotropic Light Absorption by Localized Surface Plasmon Resonance in a Thin Film of Gold Nanoparticles Studied by Visible Multiple-Angle Incidence Resolution Spectrometry, *Phys. Chem. Chem. Phys.*, **13**, 9691-9696 (2011).

Muro, M.; Itoh, Y.; Hasegawa, T., A Conformation and Orientation Model of the Carboxylic Group of Fatty Acids Dependent on Chain Length in a Langmuir Monolayer Film Studied by Polarization-Modulation Infrared Reflection Absorption Spectroscopy, *J. Phys. Chem. B*, **114**, 11496-11501 (2010).

Sakabe, T.; Yamazaki, S.; Hasegawa, T., Analysis of Cross-Section Structure of a Polymer Wrapping Film Using Infrared Attenuated Total Reflection Imaging Technique with an Aid of Chemometrics, *J. Phys. Chem. B*, **114**, 6878-6885 (2010).

Karino, Y.; Matubayasi, N., Free-energy Analysis of Hydration Effect on Protein with Explicit Solvent: Equilibrium Fluctuation of Cytochrome *c*, *J. Chem. Phys.*, **134**, 041105-041108 (2011).

Sakuraba, S.; Matubayasi, N., Distribution-function Approach to Free Energy Computation, *J. Chem. Phys.*, **135**, 114108-114118 (2011).

Takahashi, H.; Maruyama, K.; Karino, Y.; Morita, A.; Nakano, M.; Jungwirth, P.; Matubayasi, N., Energetic Origin of Proton Affinity to the Air/Water Interface, *J. Phys. Chem. B*, **115**, 4745-4751 (2011).

Molecular Fine-Structure Analysis in a Monolayer at the Air/Water Interface

When a Langmuir-adsorbed monolayer film on water (L film) of a fatty acid is studied, L-film specific factors should be taken into account as well as the chain-length dependence; i.e. strong interactions with the water surface. In an L film of a fatty acid, the carboxylic group is considered to be in deep contact with the water surface, and hydration of the carboxylic group is therefore an inevitable factor to understand the character and structure of the L film.

To study the structures of both hydrocarbon chains and the carboxylic groups, infrared (IR) spectroscopy is powerful. To prevent the disturbance by water vapor, the technique of polarization-modulation infrared reflection absorption spectroscopy (PM-IRRAS) provides a convenient way to access the fingerprint region of IR spectra of L films.

In our study, the conformation of the carboxylic group of fatty acids in a Langmuir (L) monolayer film on water was described in relation to the aggregation property of the hydrocarbon chain. Polarization-modulation infrared reflection absorption spectra (PM-IRRAS) of L films of heptadecanoic acid (C17), octadecanoic acid (C18) and nonadecanoic acid (C19) exhibited systematic spectral changes in both the C–H and C=O stretching vibration regions. Through a stabilization analysis of the L films at a high surface pressure, C19 L film has been found outstandingly stable exhibiting no film shrink, while the rest two compounds exhibit a large shrink at the high surface pressure. By taking into account the uniquely high aggregation property of the hydrocarbon chains of C19, the three major bands arising from the C=O stretching vibration mode propose three types of molecular conformations about the carboxylic group, which were elucidated by a balance of the hydration of the carboxylic group, the chain length of the hydrocarbon chain and the surface pressure.

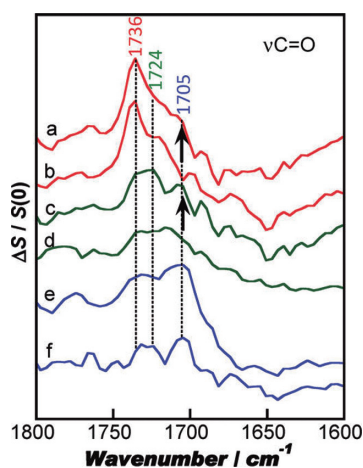


Figure 1. PM-IRRAS spectra of Langmuir monolayers of fatty acids with three different chain lengths (C17~C19) as a function of surface pressure in the C=O stretching vibration region.

Energetic Origin of Proton Affinity to the Air/Water Interface

The affinity of the hydronium ion to the air/water interface is an issue recently studied intensively by both experimental and theoretical approaches. To investigate the mechanism responsible for the surface propensity of this ion, we performed a series of novel quantum-mechanical/molecular-mechanical simulations combined with the energy-representation theory of solutions. The solvation free energy of the H_3O^+ solute placed at the interface was obtained as -98 kcal/mol, being more stable by 4 kcal/mol than in the bulk. We further decomposed the solvation free energies into contributions from the water molecules residing in the oxygen and the hydrogen sides of the solute, as shown in Figure 2, to clarify the origin of the surface preference. When the solute was displaced from the bulk to the interface, it was shown that the free energy contribution from the oxygen side is destabilized by ~ 10 kcal/mol because of a reduction of the number of surrounding solvent water molecules. It was observed, however, that the free energy contribution from the hydrogen side is unexpectedly stabilizing and surpasses the destabilization in the opposite side. We found that the stabilization in the hydrogen side originates from the solute-solvent interaction in the medium range beyond the nearest neighbor. It was also revealed that the solute's electronic polarization amounts to half the stabilization free energy change associated with the solute displacement from the bulk to the interface.

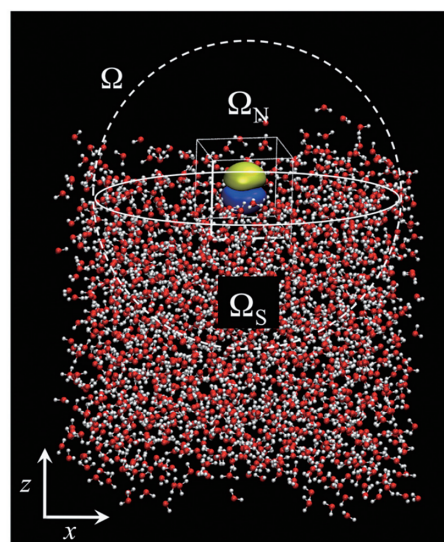


Figure 2. A QM/MM snapshot for the hydronium ion placed at $z=-2.0$ Å. The north and south hemispheres, Ω_N and Ω_S , are also presented. The cubic box in the Figure indicates the real-space grid cell to enclose the wave function of the QM solute. The yellow and the blue surfaces represent the positive and negative isosurfaces for the HOMO of the solute with the values of ± 0.001 a.u., respectively.

Division of Environmental Chemistry – Molecular Microbial Science –

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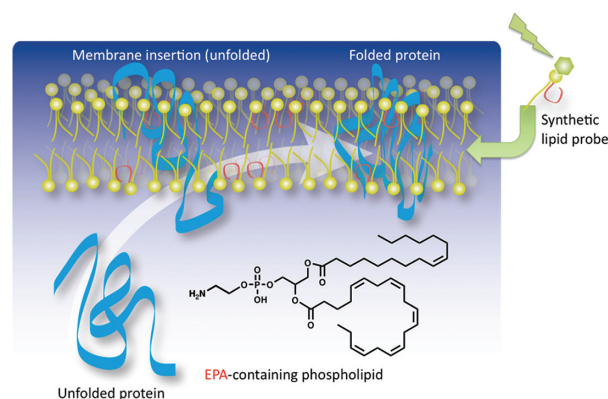
Scope of Research

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

KEYWORDS

Molecular Microbial Science
Biochemistry
Psychrotroph

Polyunsaturated Fatty Acid
Bioengineering



Selected Publications

Kawamoto, J.; Sato, T.; Nakasone, K.; Kato, C.; Mihara, H.; Esaki, N.; Kurihara, T., Favourable Effects of Eicosapentaenoic Acid on the Late Step of the Cell Division in a Piezophilic Bacterium, *Shewanella violacea* DSS12, at High-Hydrostatic Pressures, *Environ. Microbiol.*, **13**, 2293-2298 (2011).

Sato, S. B.; Sato, S.; Kawamoto, J.; Kurihara, T., Differential Roles of Internal and Terminal Double Bonds in Docosahexaenoic Acid: Comparative Study of Cytotoxicity of Polyunsaturated Fatty Acids to HT-29 Human Colorectal Tumor Cell Line, *Prostaglandins Leukot. Essent. Fatty Acids*, **84**, 31-37 (2011).

Usui, K.; Hiraki, T.; Kawamoto, J.; Kurihara, T.; Nogi, Y.; Kato, C.; Abe, F., Eicosapentaenoic Acid Plays a Role in Stabilizing Dynamic Membrane Structure in the Deep-Sea Piezophile *Shewanella violacea*: A Study Employing High-Pressure Time-Resolved Fluorescence Anisotropy Measurement, *Biochim. Biophys. Acta*, (2011) (in press).

Vasudevan, A.; Fujita, M.; Kurata, A.; Kawamoto, J.; Esaki, N.; Kurihara, T., Function of FADH₂-Dependent 2-Haloacrylate Hydratase from a 2-Chloroacrylate-Utilizing Bacterium, *Burkholderia* sp. WS, *Trace Nutrients Research*, **28**, 58-64 (2011).

Hidese, R.; Mihara, H.; Kurihara, T.; Esaki, N., *Escherichia coli* Dihydropyrimidine Dehydrogenase Is a Novel NAD-Dependent Heterotetramer Essential for the Production of 5,6-Dihydrouracil, *J. Bacteriol.*, **193**, 989-993 (2011).

Eicosapentaenoic-Acid-Containing Phospholipids Act as a Chemical Chaperone for the Rapid Folding of a Cold-Inducible-Membrane Protein

A cold-adapted microorganism, *Shewanella livingstonensis* Ac10 isolated from Antarctic seawater, produces eicosapentaenoic acid (EPA) as an acyl chain of its membrane phospholipids at 4°C. When EPA-biosynthesis genes were disrupted, the EPA-lacking mutant showed the growth retardation and formed filamentous cells at 4°C, but not at 18°C, suggesting that EPA-containing phospholipids have an important role in the cold adaptation of this bacterium. We also found that, in the EPA-lacking mutant grown at 4°C, a cold-inducible outer membrane protein, Omp74, forms different conformation from that in the parent strain. In order to elucidate the physiological role of EPA in the folding of Omp74, we performed *in vitro* reconstitution of recombinant Omp74 with the liposomes containing or not containing EPA and analyzed the effect of the presence of EPA on the folding of Omp74. The larger amounts of folded Omp74 were observed in the liposomes containing EPA than those without EPA. Circular dichroism analysis indicated that Omp74 rapidly interacts with the membrane surface and rearranges its β -sheet structures in the EPA-containing liposome at 4°C. These results suggest that EPA-containing phospholipids accelerate the secondary structure formation and folding of Omp74 and play a role as a molecular chaperone of Omp74 at low temperatures.

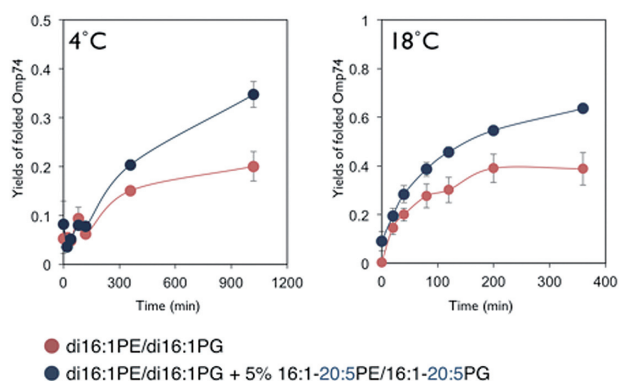


Figure 1. EPA-containing phospholipids induce the folding of a cold-inducible porin, Omp74, at low temperatures.

Studies on the Transport and Metabolism of Selenium in Mammalian Cells

Selenide is a precursor of selenophosphate, which is the active selenium donor compound required by bacteria and mammals for the synthesis of selenocysteine in selenoproteins. Although selenite is the main source for selenide, selenite reduction pathway is still largely unclear. It has been suggested that selenite is reduced by glutathione (GSH) and thioredoxin reductase (TrxR). However, these pathways have not been demonstrated in living cells. Especially, selenoprotein biosynthesis was not affected by knock down of TrxR. In this study, we evaluated the physiological role of GSH in selenoprotein biosynthesis by using hep1-6 cells. When we used buthionine sulphoximine (BSO), a selective GSH depleting agent, decrease in the production of selenoproteins was not observed. On the other hand, under the same conditions, the amounts of intracellular selenium compounds were increased. These results revealed the presence of unknown pathway for the intracellular selenium reduction. In order to explore a new mechanism for selenite reduction, we focused on glutathione reductase (GR), a homolog of TrxR, and analyzed its selenite-reducing activity *in vitro*, demonstrating that hydrogen selenide is generated as NADPH decreases under anaerobic conditions. This finding raises the possibility that GR is involved in the *in vivo* selenite reduction pathway.

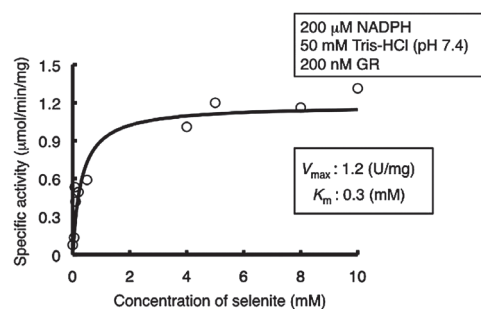


Figure 2. Selenite reducing activity of glutathione reductase (GR).

Division of Multidisciplinary Chemistry – Polymer Materials Science –

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



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Dr JENG, U-Ser National Synchrotron Radiation Research Center, Hsinchu, Taiwan, 30 May

Scope of Research

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

KEYWORDS

Polymer Physics Scattering
Polymer Properties Neutron Scattering



Selected Publications

Kawabata, J.; Matsuba, G.; Nishida, K.; Inoue, R.; Kanaya, T., Melt Memory Effects on Recrystallization of Polyamide 6 Revealed by Depolarized Light Scattering and Small-Angle X-ray Scattering, *J. Appl. Polym. Sci.*, **122**, 1913-1920 (2011).
Masunaga, H.; Ogawa, H.; Takano, T.; Sasaki, S.; Goto, S.; Tanaka, T.; Seike, T.; Takahashi, S.; Takashita, K.; Nariyama, N.; Ohashi, H.; Ohta, T.; Furukawa, Y.; Matsushita, T.; Ishizawa, Y.; Yagi, N.; Takata, M.; Kitamura, H.; Sakurai, K.; Tashiro, K.; Takahara, A.; Amamiya, Y.; Horie, K.; Takenaka, M.; Kanaya, T.; Jinnai, H.; Okuda, H.; Akiba, I.; Takahashi, I.; Yamamoto, K.; Hikosaka, M.; Sakurai, S.; Shinohara, Y.; Okuda, A.; Sugihara, Y., Multipurpose Soft-Material SAXS/WAXS/GISAXS Beamline at SPring-8, *Polymer Journal*, **43**, 1-7 (2011).
Asakawa, H.; Nishida, K.; Matsuba, G.; Kanaya, T.; Ogawa, H., Crystallization of Isotactic Polypropylene from Mesomorphic Phase: A Constant Heating Rate Study, *Journal of Physics: Conf. Ser.*, **272**, [012024-1]-[012024-4] (2011).
Inoue, R.; Kawashima, K.; Matsui, K.; Nakamura, M.; Nishida, K.; Kanaya, T.; Yamada, N. L., Interfacial Properties of Polystyrene Thin Films as Revealed by Neutron Reflectivity, *Phys. Rev.*, **E84**, [031802-1]- [031802-7] (2011).
Nishida, K.; Okada, K.; Asakawa, H.; Matsuba, G.; Ito, K.; Kanaya, T.; Kaji, K., In Situ Observations of the Mesophase Formation of Isotactic Polypropylene -A Fast Time-resolved X-ray Diffraction Study, *Polymer Journal*, **44**, 95-101 (2012).

Precursor of Shish-kebab by Micro-beam WAXS

It is well known that when semi-crystalline polymers are crystallized under shear flow or elongational flow the so-called shish-kebab structure is formed. It is considered that the shish-kebabs consist of extended chain crystals (shish) and folded chain lamella crystals (kebab) grown on the extended chain crystals. It is believed that the shish-kebab is a structure basis of ultra-high modulus and ultra-high strength fiber, and hence many studies have been performed on the shish-kebab. One of the recent topics in the field is precursor of the shish-kebab. In order to understand the role of the precursor we studied structure formation process of isotactic polystyrene (iPS) after applying pulse shear above the nominal melting temperature T_m using depolarized light scattering (DPLS), polarized optical microscope (POM) and small- and wide angle scattering (SAXS, WAXS), and found that precursors were formed in μm scale above T_m . Although we did not observe any signs of crystals in normal WAXS measurements, we could not reach a final conclusion that the precursors did not include crystals. In this work inner structure of the precursor of iPS was studied above T_m using *micro-beam WAXS*. The result of *micro-beam WAXS* mapping on the precursor is shown in Figure 1. Symbols or no symbols in the mapping area indicate that we could observe the Bragg diffractions or no Bragg diffractions (see also Figure 2), showing that the precursor certainly includes crystallites which can survive at temperatures even above the nominal melting temperature.

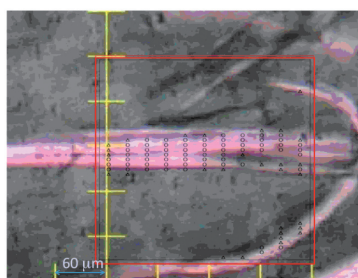


Figure 1. POM image of precursor of iPS for micro-beam WAXS mapping.

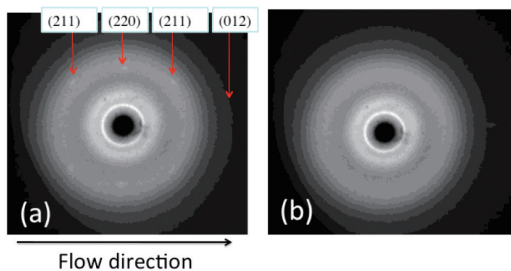


Figure 2. Micro-beam diffraction patterns. (a) beam is on the precursor, (b) beam is out of precursor.

Fast Time-Resolved X-Ray Scattering Measurements of Mesophase Formation of Isotactic Polypropylene

Isotactic polypropylene (iPP) has a mesophase, besides major three kinds of crystalline modifications, such as alpha-, beta- and gamma-forms. Mesophase iPP in appearance is transparent like a glassy polymer and the structure in wide-angle X-ray diffraction (WAXD) scale is intermediate one between amorphous and crystal. In small-angle X-ray scattering (SAXS) scale, the mesophase iPP is characterized by the so-called “nodule” of spherical or polygonal shape with the diameter of ca. 10 nm. The mesophase iPP is obtained empirically by dropping thin molten iPP rapidly into ice water. Namely, the formation speed of the mesophase iPP is particularly high and the formation process finishes for a short period of time. Even so, ex-situ preparation of the mesophase iPP is rather readily achieved; accordingly the finished form of the mesophase iPP from various viewpoints has been extensively studied so far. However, in-situ observation of the formation process of the mesophase iPP during such a short period has been a challenging issue up to the present. Combining effectively a rapid temperature-jump technique and a synchrotron radiation X-ray scattering technique, we have accomplished in-situ WAXD and SAXS observations during the rapid cooling of iPP from molten state.

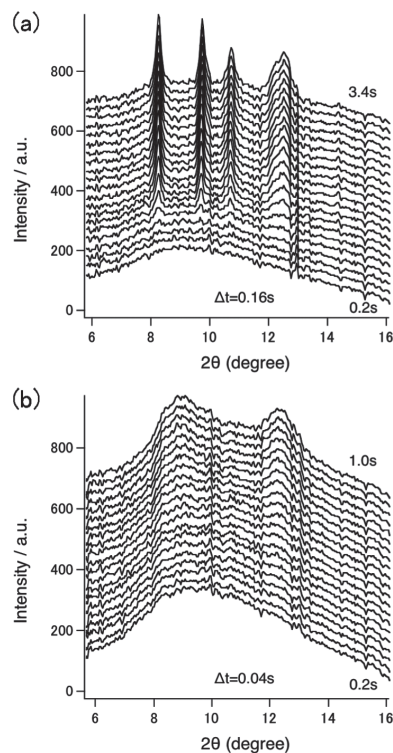


Figure 3. Time evolution of WAXD profiles during the molten iPP is rapidly cooled to (a) 80°C and (b) -10°C.

Division of Multidisciplinary Chemistry – Molecular Rheology –

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



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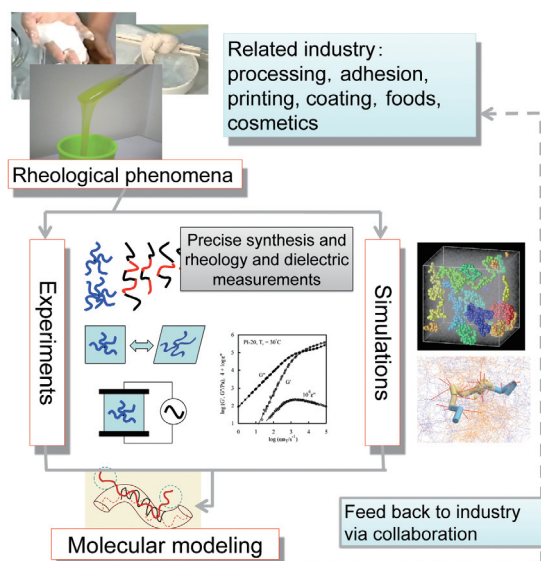
Sungkyunkwan University, Korea, R., 1 April–30 September
Technical University of Athens, Greek, 7–12 September
Technische Universität Darmstadt, Germany, 23 September
University of Naples, Italy, 18 March–27 April

Scope of Research

The molecular origin of various rheological properties of material is studied. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For basic understanding of the features, the molecular motion and structures at various scales are studied for polymeric systems in deformed state. Measurements are performed of rheological properties with various rheometers, of isochronal molecular orientation with flow birefringence, and of auto-correlation of the orientation with dynamic dielectric spectroscopy. Direct observation of molecular motion is also carried out with fluorescent microscopy and molecular simulations.

KEYWORDS

Rheology Polymers Suspensions
Softmatters Emulsions



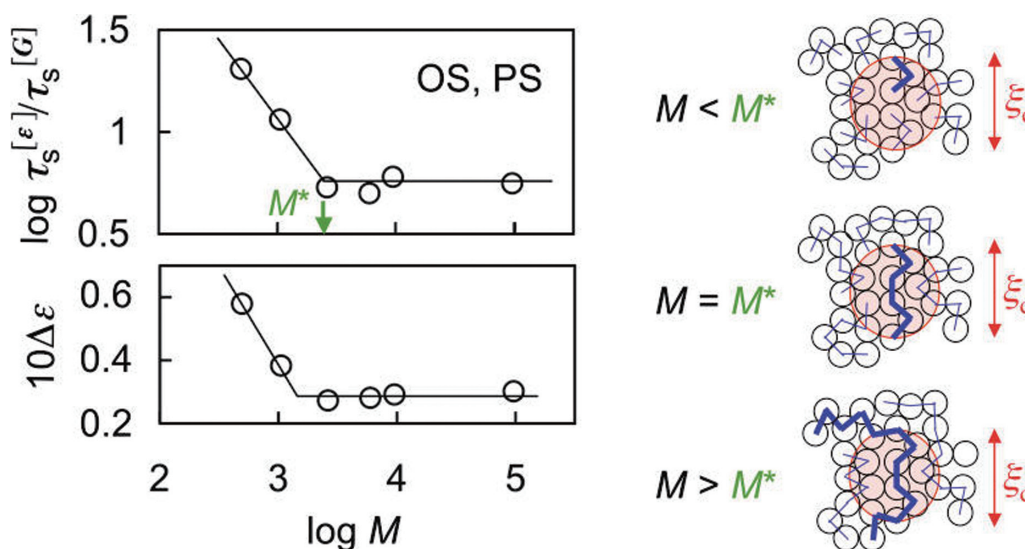
Selected Publications

- Watanabe, H.; Chen, Q.; Kawasaki, Y.; Matsumiya, Y.; Inoue, T.; Urakawa, O., Entanglement Dynamics in Miscible Polyisoprene/Poly(*p*-tert-butylstyrene) Blends, *Macromolecules*, **44**(6), 1570-1584 (2011).
- Matsumiya, Y.; Uno, A.; Watanabe, H.; Inoue, T.; Urakawa, O., Dielectric and Viscoelastic Investigation of Segmental Dynamics of Polystyrene above Glass Transition Temperature: Cooperative Sequence Length and Relaxation Mode Distribution, *Macromolecules*, **44**(11), 4355-4365 (2011).
- Uneyama, T.; Horio, K.; Watanabe, H., Anisotropic Mobility Model for Polymers under Shear and Its Linear Response Functions, *Phys. Rev. E*, **83**(6), 061802 (2011).
- Masubuchi, Y.; Yaoita, T.; Matsumiya, Y.; Watanabe, H., Primitive Chain Network Simulations for Asymmetric Star Polymers, *J. Chem. Phys.*, **134**, [194905-1]-[194905-7] (2011).
- Watanabe, H., Slow Dynamics in Homopolymer Liquids, *Polym. J.*, **41**(11), 929-950 (2009).

Dielectric and Viscoelastic Investigation of Segmental Dynamics of Polystyrene above Glass Transition Temperature: Cooperative Sequence Length and Relaxation Mode Distribution

Atactic polystyrene (PS) has the type-B dipole perpendicular to the chain backbone so that its segmental motion activates the dielectric relaxation. For monodisperse PS and oligostyrene (OS) samples of various molecular weights M , details of this motion were examined at temperatures T well above T_g through comparison of the complex modulus, $G^*=G'+iG''$, and the complex dielectric permittivity, $\epsilon^*=\epsilon'-i\epsilon''$, measured as functions of the angular frequency ω . For the OS samples, $G^*(\omega)$ and $\epsilon^*(\omega)$ fully relaxed through the segmental dynamics thereby exhibiting low- ω terminal tails, $G'(\omega)\propto\omega^2$, $G''(\omega)\propto\omega$, $\Delta\epsilon'(\omega)\equiv\epsilon'(0)-\epsilon'(\omega)\propto\omega^2$, and $\epsilon''(\omega)\propto\omega$, at ω below the segmental relaxation frequency ω_s . For the PS samples, $G^*(\omega)$ relaxed partly through the segmental dynamics and then exhibited the polymeric full relaxation characterized by the Rouse-like behavior followed by the terminal flow behavior (with/without intermediate entanglement plateau depending on M). In contrast, $\epsilon^*(\omega)$ of the PS samples still relaxed completely through the segmental dynamics. For respective samples, the $G^*(\omega)$ and $\epsilon^*(\omega)$ data in the segmental

relaxation zone exhibited very similar relaxation mode distribution. Nevertheless, a ratio of the dielectrically and viscoelastically detected segmental relaxation times, $r(M)=\omega_{s,G}/\omega_{s,\epsilon}$, and the dielectric relaxation intensity, $\Delta\epsilon(M)$, decreased with increasing M up to $M^*\cong 2\times 10^3$ and then became insensitive to M on a further increase of M . The viscoelastic segmental relaxation reflects the cooperative torsion of the repeating units along the molecular backbone, while the dielectric segmental relaxation detects reorientational motion of those units affected by both intra- and inter-molecular cooperativity. The observed decreases of $r(M)$ and $\Delta\epsilon(M)$ suggested that the dimension ζ_m of the whole OS molecule (over which the cooperative torsion occurs) is smaller than the length scale ζ_c for the inter-molecular cooperative motion and that ζ_m approaches ζ_c on an increase of M up to M^* . Consequently, the high- M PS molecules having $\zeta_m>\zeta_c$ exhibited the M -insensitive $r(M)$ and $\Delta\epsilon(M)$. Thus, the M value for the crossover between these two regimes, $M^*\cong 2\times 10^3$, can be taken as the molecular weight of the cooperative sequence along the PS backbone. Furthermore, the quantitative similarity of the viscoelastic and dielectric mode distributions suggests that the cooperative torsion of the repeating units along the molecular backbone is governed by the cross-correlation of the units belonging to different molecules.



Division of Multidisciplinary Chemistry – Molecular Aggregation Analysis –

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



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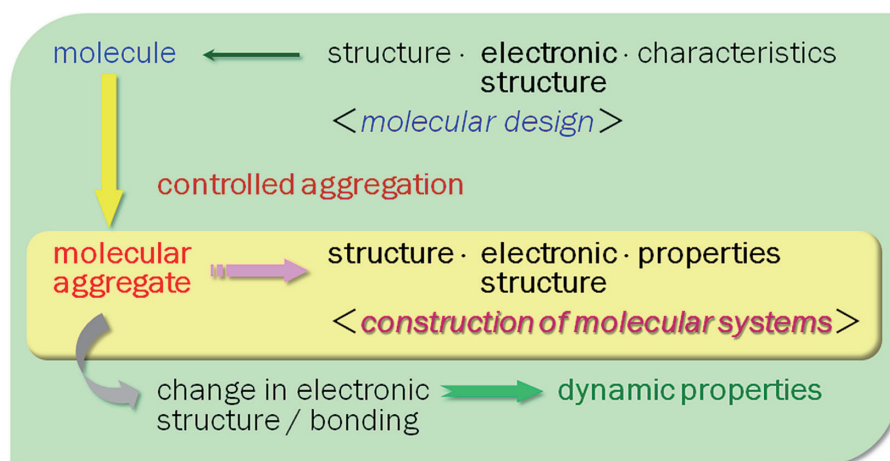
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Scope of Research

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

KEYWORDS

Cultured Cell
Dielectric Monitoring
Photoinduced Decay
Surface Potential
Zwitterionic Molecule



Selected Publications

Tsutsumi, J.; Yoshida, H.; Murdey, R.; Sato, N., Decay Mechanism of Spontaneously Built-up Surface Potential in a Thin Film of a Zwitterionic Molecule Having Noncentrosymmetric Crystal Structure, *J. Phys. Chem. C*, **115**, 2356-2359 (2011).

Yoshida, H.; Sato, N., The Depth Profile of Core Energy Levels: Electronic Structure of Buried Organic/Metal Interfaces Examined by X-Ray Photoemission and Target Factor Analysis, *Chem. Phys. Lett.*, **511**, 146-150 (2011).

Murdey, R.; Sato, N., *In Situ* Conductance Measurements of Copper Phthalocyanine Thin Film Growth on Sapphire [0001], *J. Chem. Phys.*, **134**, [234702-1]-[234702-5] (2011).

Asami, K., Dielectric Properties of Microvillous Cells Simulated by the Three-Dimensional Finite-Element Method, *Bioelectrochemistry*, **81**, 28-33 (2011).

Asami, K., Design of a Measurement Cell for Low-Frequency Dielectric Spectroscopy of Biological Cell Suspensions, *Meas. Sci. Technol.*, **22**, [085801-1]-[085801-7] (2011).

Decay Mechanism of Spontaneously Built-up Surface Potential in a Thin Film of a Zwitterionic Molecule Having Noncentrosymmetric Crystal Structure

The photoinduced decay of spontaneously built-up surface potential was investigated for a vacuum-deposited polycrystalline thin film of a zwitterionic molecule, pyridinium 5,7-dihydro-5,7-dioxo-6*H*-cyclopenta[*b*]pyridin-6-ylide (4N-PI) (Figure 1). The excitation energy required to induce the decay lies above the energy gap of 2.2 eV in accordance with the photoconduction threshold. Using fixed excitation energy of 2.8 eV, the decay rate was examined for two films for which different crystallinity was observed and it turned out to increase with increasing film crystallinity. Besides, photoinduced decay of the surface potential has also been observed for Alq₃. However, two different mechanisms are proposed to explain this behavior. One is the relaxation of preferentially ordered molecular dipole moments by photoinduced molecular rotation, and the other is cancellation of the built-up potential through the displacement of photogenerated charge carriers. To our knowledge, there is no conclusion to this controversy, especially with due consideration of the high molecular symmetry of Alq₃. In this work the current-voltage relationship obtained from the surface potential decay for 4N-PI is found to be explained by a combination of an ohmic behavior at low voltages and a trap-limited space-charge-limited-current conduction at high voltages. The electrical parameters derived from the fitted *I-V* curves trend appropriately with the change in film crystallinity. We therefore conclude that photogenerated carriers, rather than molecular rotations, contribute essentially to the disappearance of the surface potential of 4N-PI films under illumination.

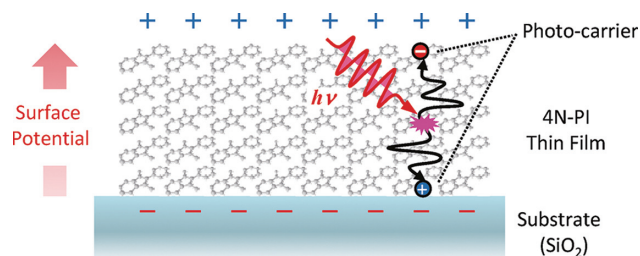


Figure 1. Schematic of photoinduced decay of spontaneously built-up surface potential for a vacuum-deposited polycrystalline thin film of pyridinium 5,7-dihydro-5,7-dioxo-6*H*-cyclopenta[*b*]pyridin-6-ylide (4N-PI).

Dielectric and Optical Monitoring of Animal Cells Cultured on ITO Transparent Electrode

Cultured cells are commonly used for screening of toxicants and medicines. The screening requires high sensitive, high throughput and inexpensive sensing techniques. Dielectric spectroscopy would be a feasible tool for the screening because it is sensitive to the morphology and electrical properties of cells as well as a label-free and noninvasive method. In this study, we have developed a real-time dielectric monitoring system where cells are cultured on ITO-coated glass plates, which permit simultaneous observation of cells by optical microscopy. Electric admittance between the ITO electrode and the Pt electrode placed in the culture medium was measured at a regular interval. With the confluent monolayers of Mardin-Darby canine kidney cells, which are connected to each other with tight junctions, effects of apoptosis inducers (camptothecin (CT), actinomycin D (AD) and cycloheximide (CH)) were examined (Figure 2). Several hours after the dosage, the conductance of the cell monolayer increased, accompanied by appearance of gaps between cells, i.e., opening of tight junctions. At the final stage, all cells became spherical and separated from the ITO electrode, being electrically invisible. The results suggest that the dielectric monitoring technique is a promising tool for sensing the morphological changes of cells in response to toxicants and medicines.

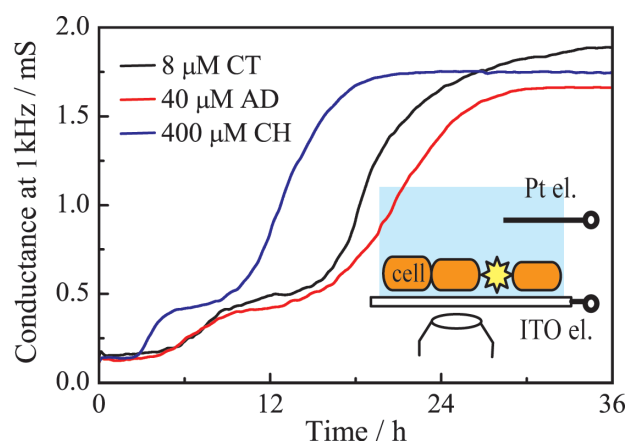


Figure 2. Conductance changes of the cell culture system (inset) after dosage of apoptosis inducers.

Division of Multidisciplinary Chemistry – Interdisciplinary Chemistry for Innovation –



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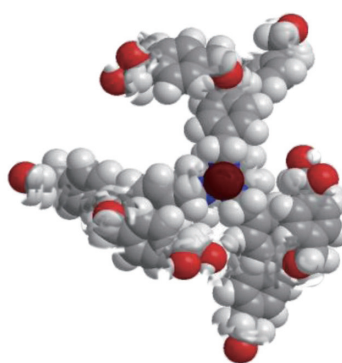
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UMEMURA, Takashi (UG)
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Scope of Research

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



KEYWORDS

Innovation
Organic Synthesis
Heteroatom Chemistry
Transition Metal Catalyst
Asymmetric Synthesis



Selected Publications

- Kondo, T.; Kimura, Y.; Kanda, T.; Takagi, D.; Wada, K.; Toshimitsu, A., Simple and Practical Aerobic Oxidation of Alcohols Catalyzed by a (μ -Oxo)tetraruthenium Cluster, *Green Sus. Chem.*, (in press).
- Kondo, T.; Niimi, M.; Yoshida, Y.; Wada, K.; Mitsudo, T.; Kimura, Y.; Toshimitsu, A., Rhodium-catalyzed Linear Codimerization and Cycloaddition of Ketenes with Alkynes, *Molecules*, **15**, 4189-4200 (2010).
- Sakanoue, T.; Yahiro, M.; Adachi, C.; Takimiya, K.; Toshimitsu, A., Electrical Characteristics of Single-component Ambipolar Organic Field-effect Transistors and Effects of Air Exposure of Them, *J. Appl. Phys.*, **103**, [094509-1]-[094509-6] (2008).
- Sakanoue, T.; Yahiro, M.; Adachi, C.; Uchiuzou, H.; Takahashi, T.; Toshimitsu, A., Ambipolar Light-emitting Organic Field-effect Transistors Using a Wide-band-gap Blue-emitting Small Molecule, *Appl. Phys. Lett.*, **90**, [171118-1]-[171118-3] (2007).
- Okamoto, K.; Nishibayashi, Y.; Uemura, S.; Toshimitsu, A., Asymmetric Carboselenation of Olefins with Aromatic Compounds, *Angew. Chem. Int. Ed. Engl.*, **44**, 3588-3591 (2005).

One-pot Synthesis of Rhodanines from Ketenes and Isothiocyanates Using Rhodium Catalyst

Rhodanines are highly important heterocyclic compounds used in the medical inspection of copper in liver, the metal-free dye-sensitized solar cell, and so on. However, the synthetic methods reported so far are limited to the multistep reactions. We succeeded in one-pot synthesis of rhodanines from ketenes and isothiocyanates using rhodium catalyst. Thus, by the reaction of phenylethylketene (2.5 mmol) and ethylisothiocyanate (1 mmol) in demethylacetamide as solvent in the presence of $[\text{RhCl}(\text{cod})]_2$ (0.0025 mmol) and dppb (0.005 mmol) at 80°C for 12 h, the rhodanine bearing phenyl and ethyl groups are produced in 99% yield (Figure 1).

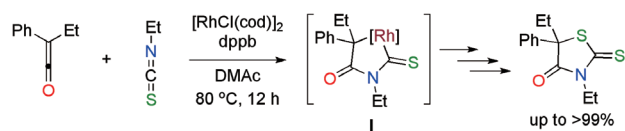
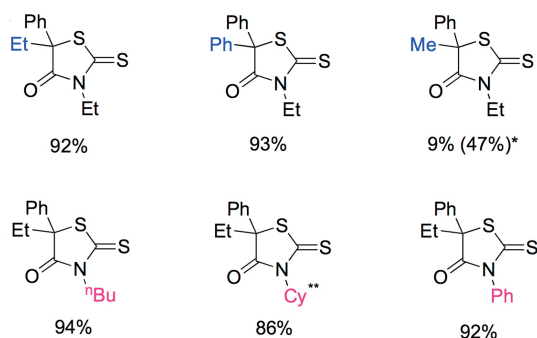


Figure 1. Synthesis of Rhodanine Derivatives.

It should be noted that one sulphur atom incorporated in the ring derives from second molecule of isothiocyanate with the elimination of isonitrile. The initial step of this reaction is expected to be the formation of rhodacyclic intermediate such as (1). Coordination of another isothiocyanate, followed by insertion of the C=S group into (1), dissociation of an isonitrile, and reductive elimination would afford the corresponding rhodanine.

Typical examples are summarized in Figure 2.



*Isothiocyanate was used in excess. **Cyclohexyl

Figure 2. Synthesis of Various Rhodanines.

Simple and Practical Aerobic Oxidation of Alcohols Catalyzed by Rhodium Cluster

The selective oxidation of primary and secondary alcohols to the corresponding aldehydes and ketones, respectively, is a ubiquitous and pivotal reaction in organic synthesis and the chemical industry. Such oxidation reactions have been performed traditionally using stoichiometric amount of inorganic oxidants, such as CrO_3 , KMnO_4 , MnO_2 , and SeO_2 . However, these oxidation methods have serious drawbacks, such as their cost and the production of environmentally hazardous/toxic byproducts. From both economic and environmental viewpoints, there is an urgent demand for greener, more atom-efficient methods that use O_2 and *air* as readily available terminal and ideal oxidants, and produce only H_2O as a byproduct.

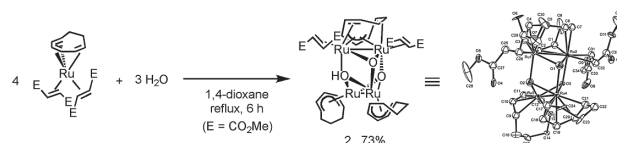


Figure 3. Synthesis of Catalyst.

We have found that the (μ -oxo)tetraruthenium cluster (2), prepared by the method shown in Figure 3, efficiently catalyzes a simple, practical, and selective oxidation of primary and secondary alcohols to the corresponding aldehydes and ketones, respectively, under 1 atm of O_2 or air. For example, in the presence of 2 (0.005 mmol), benzyl alcohol (1 mmol) was smoothly oxidized in *N,N*-dimethylacetamide (DMA) at 80°C for 20 h under 1 atm of O_2 (balloon) to give benzaldehyde in 95% yield (Figure 4).

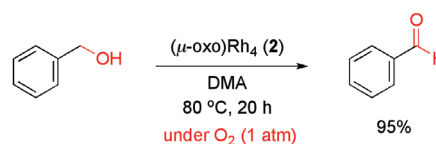


Figure 4. Oxidation of Alcohols.

Neither benzoic acid nor acetal of benzaldehyde was obtained at all. In the case of secondary alcohol, it was necessary to carry out the reaction at 130°C. At this condition, benzophenone was obtained quantitatively by the aerobic oxidation of diphenylmethanol.

After the reactions, 2 was recovered in 20% yield by simple column chromatography. In addition, mononuclear $\text{Ru}(\eta^6\text{-cot})(\eta^2\text{-dmfm})_2$, which is the starting material for the synthesis of 2, showed no catalytic activity in either the absence or presence of a small amount of H_2O . These results strongly suggest that tetraruthenium cluster (2) acts as an active catalytic species throughout the reaction.

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Scope of Research

The Following Subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Ultra-low Emittance state of a proton beam created by the electron cooling: Laser cooling of Mg^+ ion beam: Irradiation of short bunch proton beam by electron cooling and phase rotation: Research and development of permanent quadrupole magnets for final focusing of International Linear Collider(ILC): Development of electron-cyclotron resonance(ECR) ion source for small neutron source.

KEYWORDS

Beam Physics
Accelerator Physics
Beam Cooling
Phase Rotation
Neutron Optics

Selected Publications

Noda, A., Ion Beam Cooling at S-LSR Project, *Nucl. Instrum. Meth.*, **A532**, 150-156 (2004).

Shirai, T.; Ikegami, M.; Fujimoto, S.; Souda, H.; Tanabe, M.; Tongu, H.; Noda, A.; Fujimoto, T.; Iwata, S.; Shibuya, S.; Smirnov, A.; Meshkov, I.; Fadil, H.; Grieser, M., One Dimensional Beam Ordering of Protons in a Storage Ring, *Phys. Rev. Lett.*, **98**, [204801-1]-[204801-4] (2007).

Nakamura, S.; Ikegami, M.; Iwashita, Y.; Shirai, T.; Tongu, H.; Souda, H.; Daido, H.; Mori, M.; Kado, M.; Sagisaka, A.; Ogura, K.; Nishiuchi, M.; Orimo, S.; Hayashi, Y.; Yogo, A.; Pirozhkov, A. S.; Buranov, S. V.; Esirkepov, T.; Nagashima, A.; Kimura, T.; Tajima, T.; Takeuchi, T.; Fukumi, A.; Li, Z.; Noda, A., High-Quality Laser-Produced Proton Beam Realized by the Application of a Synchronous RF Electric Field, *Jpn. J. Appl. Phys.*, **46**, L717-L720 (2007).

Wakasugi, M.; Emoto, T.; Furukawa, Y.; Ishii, K.; Ito, S.; Koseki, T.; Kurita, K.; Kuwajima, A.; Masuda, T.; Morikawa, A.; Nakamura, M.; Noda, A.; Ohnishi, T.; Shirai, T.; Suda, T.; Takeda, H.; Tamae, T.; Tongu, H.; Wang, A.; Yano, Y., Novel Internal Target for Electron Scattering Off Unstable Nuclei, *Phys. Rev. Lett.*, **100**, [164801-1]-[164801-4] (2008).

Iwashita, Y.; Tajima, Y.; Hayano, H., Development of High Resolution Camera for Observations of Superconducting Cavities, *Phys. Rev. S.T.-Accel. Beams*, **11**, [093501-1]-[093501-6] (2008).

Approach to High Efficiency Indirect Transverse Laser Cooling

At S-LSR, a laser cooling has been applied to $^{24}\text{Mg}^+$ ions in order to realize a crystalline beam with the use of a very strong cooling force of laser cooling. Cooling in the longitudinal direction has already been attained for both a coasting beam and a bunched beam. Indirect transverse laser cooling by synchro-betatron coupling [1] has also been demonstrated as shown in Figure 1, the cooling efficiency of which, however, was found to be not so high as enables the crystalline beam getting over the hill of heating force due to Intra-Beam Scattering (IBS) (Figure 2 [2]). For this purpose, it is required to reduce the beam intensity in order to suppress IBS. The reduction of the beam intensity, however, results in a deterioration of signal to noise ratio for measurements of the beam, especially for the optical measurement of spontaneous emission from laser excited Mg ions with the use of a cooled CCD in order to measure the horizontal beam size.

We are investigating the capability to reduce the beam intensity without deteriorating S/N ratio so much by "Controlled Scraping", which applies two dimensional laser cooling with the use of resonant coupling together with a time variable scraping as illustrated in Figure 3. The essential feature of this scheme is gradual reduction of beam aperture by a scraper according to the performance of horizontal beam size reduction with an indirect horizontal laser cooling using synchro-betatron resonant coupling. Recent beam experiments showed the elongation of beam life by putting a scraper closer to the beam center after application of two dimensional laser cooling.

- [1] H. Okamoto, A.M. Sessler and D. Möhl, Phys. Rev. Lett. **72**, (1994) 3977.
 [2] M. Bussmann et al., Presentation at SPARC07.

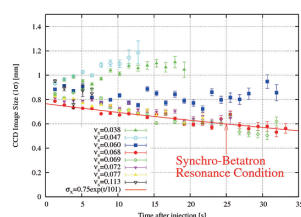


Figure 1.

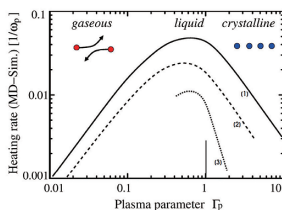


Figure 2.

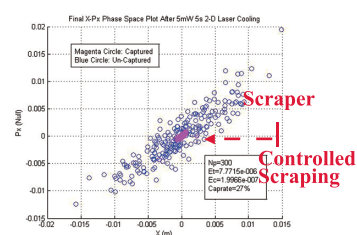


Figure 3.

Permanent Magnet Focusing for Klystrons

Applying permanent magnet technology to beam focusing in klystrons can reduce their power consumption and increase reliability. These features benefit a variety of applications especially for large facilities that use a number of klystrons such as the International Linear Collider (ILC), one of the important future projects of high energy physics. A Japanese group proposes a Distributed RF System (DRFS) to eliminate a complicated RF waveguide system, where about 4000 relatively small modulating anode (MA) klystrons will be used. Because of the large number of units, the failure rate of every component has to be minimized. A low beam voltage owing to the moderate output power and less stress to the RF window should make the lifetime of the klystrons longer. The maintenance problem caused by the large number of electromagnets and power supplies will be relaxed by replacing the electromagnets by permanent magnets, which eliminates 4000 power supplies and cooling systems. Hence the down time of the RF system can be expected to be small. The low magnetic field needed for the purpose allows us to apply inexpensive ferrite magnets instead of magnets using rare earth material. The magnet system is designed by a 3D magnetic field calculation code and fabricated at 1/2 scale. The results will be used to fabricate a full scale model for a real klystron, which will be evaluated by a power test next year.

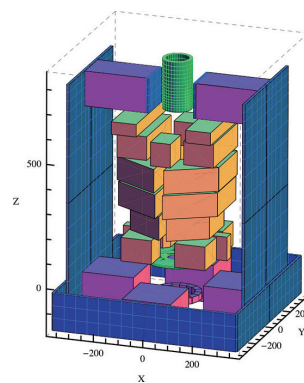


Figure 4. Permanent magnet focusing system designed with RADIA4.29.

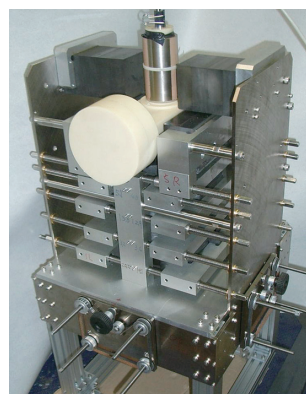


Figure 5. Fabricated half scale model of the permanent magnet focusing system. A 1/2 mockup of the klystron is inserted to check the geometry.

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Scope of Research

The interaction of femtosecond laser pulses with matters involves interesting physics, which does not appear in that of nanosecond laser pulses. Investigating the interaction physics, potential of intense femtosecond lasers for new applications is being developed (such as laser produced radiations and laser processing). Ultra-intense lasers can produce intense radiations (electrons, ions, THz, and so on), which can be expected as the next-generation radiation sources. Ultra-short lasers are available to process any matters without thermal dissociation. The femtosecond laser processing is also the next-generation laser processing. In our laboratory ultra intense femtosecond laser named T⁶-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

KEYWORDS

Intense Laser Science
Laser Plasma Radiations
(Electrons, Ions, and THz)
Ultrafast Electron Diffraction (UED)
Laser Nano-ablation Physics
Femtosecond Laser Processing
Mid-infrared Fiber Lasers

Physics of intense
femtosecond laser
matter interactions
and its applications

CPA laser technology

Fiber lasers



Intense laser plasma
interactions

Laser interactions
with clusters, surfaces etc.

Basic Physics

Processings

Laser R&D

Applications

Radiation source production and its applications

Reforming & functional-
alization of surfaces

Self-organization of periodic
grating structures
Control of the field emission
of CNT on surfaces

Fine machining of
soft matters

Processing of expanded poly-
tetra-fluoroethylene

Electrons

Demonstration of Ultrafast electron diffraction (UED)
Characterization and control of laser produced / accelerated electrons

Ions

Sheath acceleration of monoenergetic and high emittance ions
High energy ion production by Coulomb explosion of nano particles

Neutrons

Neutron generation by Coulomb explosion of clusters
Feasibility study for compact neutron sources produced by intense lasers

THz waves

THz generation from laser produced plasmas
Efficient THz generation from laser-cluster interactions

Selected Publications

Jahangiri, F.; Hashida, M.; Tokita, S.; Nagashima, T.; Hangyo, M.; Sakabe, S., Directional Elliptically Polarized Terahertz Emission from Air Plasma Produced by Circularly Polarized Intense Femtosecond Laser Pulses, *Appl. Phys. Lett.*, **99**, 161505 (2011).

Otani, K.; Tokita, S.; Nishoji, T.; Inoue, S.; Hashida, M.; Sakabe, S., Efficient Laser-proton Acceleration from an Insulating Foil with an Attached Small Metal Disk, *Appl. Phys. Lett.*, **99**, 161501 (2011).

Inoue, S.; Tokita, S.; Otani, K.; Hashida, M.; Sakabe, S., Femtosecond Electron Deflectometry for Measuring Transient Fields Generated by Laser-accelerated Fast Electrons, *Appl. Phys. Lett.*, **99**, 31501 (2011).

Tokita, S.; Murakami, M.; Shimizu, S.; Hashida, M.; Sakabe, S., 12W Q-switched Er:ZBLAN Fiber Laser at 2.8 μm , *Opt. Lett.*, **36**, 2812-2814 (2011).

Tokita, S.; Otani, K.; Nishoji, T.; Inoue, S.; Hashida, M.; Sakabe, S., Collimated Fast Electron Emission from Long Wires Irradiated by Intense Femtosecond Laser Pulses, *Phys. Rev. Lett.*, **106**, 255001 (2011).

Hashida, M.; Miyasaka, Y.; Ikuta, Y.; Tokita, S.; Sakabe, S., Crystal Structures on a Copper Thin Film with a Surface of Periodic Self-organized Nanostructures Induced by Femtosecond Laser Pulses, *Phys. Rev. B*, **83**, 235413 (2011).

Hashida, M.; Sakabe, S.; Izawa, Y., Symmetric Charge-transfer Cross Sections of IIIa Rare-earth-metal Elements, *Phys. Rev. A*, **83**, 32704 (2011).

Mechanism for Crystal Structure Transformation on Metal Surface by Femtosecond Laser Pulses

The precise measurement for crystallinity degree was performed on copper thin film with transmission electron microscope. We have analyzed the electron diffraction patterns in the laser fluence of 0.08–0.64 J/cm² where the grating structure is formed on thin films. It is found that the crystal structures are transformed depending on laser fluence; polycrystalline structures at <0.2 J/cm², amorphous at ~0.23 J/cm², and polycrystalline structures again at >0.35 J/cm². The mechanism of crystal structure transformation by femtosecond laser pulses is conceptually proposed, that is induced by the injection of energetic ions generated in the process of self-formation of periodic structures.

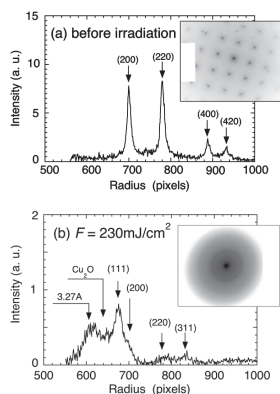


Figure 1. Electron diffraction patterns of thin Cu films (a) before irradiation and (b) at 0.23 J/cm².

Directional Elliptically Polarized THz Beam Emission from Air Plasma Produced by an Intense Femtosecond Laser Pulse

Terahertz (THz) radiation generated through the interactions of circularly polarized intense femtosecond laser pulses with air in the atmosphere has been studied. Strongly directional elliptically polarized THz emission in the forward direction is detected. The THz waves exhibits elliptical polarization with an ellipticity factor of 0–0.2 in the laser energy range of 10–50 mJ. The parametric decay of laser light to R-waves in plasma in the presence of an axial B field is proposed as a mechanism to interpret the experimental observations of the directionality, ellipticity, and energy dependence of the THz waves.

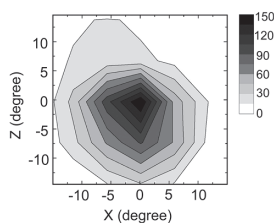


Figure 2. Typical spatial distribution of THz power emitted in forward direction for laser pulse energies of 50 mJ.

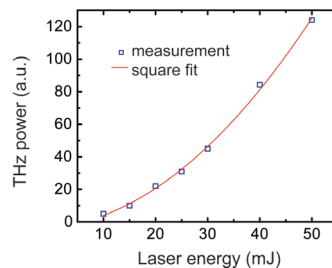


Figure 3. Laser pulse energy dependence of total THz power.

High-directivity Electron Emission from Laser-irradiated Wires

During the interaction of ultrahigh-intensity short laser pulses with solid targets, a large amount of electrons with kinetic energies of hundreds of kiloelectronvolts and higher are generated. Such electron sources have been extensively studied because of their potential applications. However, this electron source has a major problem: the electron emission generally shows little or no directivity. We have found experimentally that energetic electrons emitted from a metallic wire irradiated by an intense femtosecond laser pulse can be guided along the wire resulting in high directivity. This new electron source will be useful for many applications, because of high generation efficiency and high brightness, for instance the ultrafast electron diffraction, which needs short electron pulses in the sub-MeV energy range.

Figure 4 shows the experimental setup and results of angular distribution measurement of electrons. An imaging plate (IP) is used to detect the electrons with energies higher than 100 keV. The electrons form distinctive ring-shaped patterns on the IP. The overall size of the pattern is drastically reduced as the wire length L is increased. The FWHMs of the electron emission in the horizontal and vertical directions are as narrow as 20 and 65 mrad, respectively, at $L=30$ mm. The IP signal intensity increases with increasing the wire length: the signal intensity at the brightest spot for $L=30$ mm is 7-fold higher than that for $L=2.5$ mm. The total number of detected electrons is estimated to be of the order of 3×10^9 at $L=30$ mm.

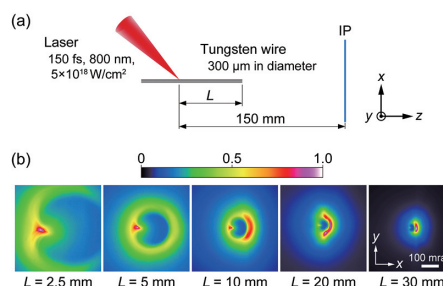


Figure 4. (a) Experimental setup for measurement of electron angular distribution. (b) Single-shot images detected by the IP. The color scale is set independently for each image for maximum contrast.

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Scope of Research

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

KEYWORDS

TEM EELS
STEM SPM
Cryo-TEM



Selected Publications

Kobayashi, T.; Ogawa, T.; Moriguchi, S.; Suga, T.; Yoshida, K.; Kurata, H.; Isoda, S., Inhomogeneous Substitution of Polyhalogenated Copper-phthalocyanine Studied by High-resolution Imaging and Electron Crystallography, *J. Electron Microsc.*, **52**, 85-90 (2003).
Minari, T.; Nemoto, T.; Isoda, S., Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor, *J. Appl. Phys.*, **99**, 034506 (2006).
Kiyomura, T.; Nemoto, T.; Ogawa, T.; Minari, T.; Yoshida, K.; Kurata, H.; Isoda, S., Thin-Film Phase of Pentacene Film Formed on KCl by Vacuum Deposition, *Jpn. J. Appl. Phys.*, **45**, 401-404 (2006).
Haruta, M.; Yoshida, K.; Kurata, H.; Isoda, S., Atomic Resolution ADF-STEM Imaging of Organic Molecular Crystal of Halogenated-Cu-phthalocyanine, *Ultramicroscopy*, **108**, 545-551 (2008).
Haruta, M.; Kurata, H.; Komatsu, H.; Shimakawa, Y.; Isoda, S., Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite $\text{La}_2\text{CuSnO}_6$, *Physical Review B*, **80**, 165123 (2009).

Local Electronic Structure Analysis for Brownmillerite $\text{Ca}(\text{Sr})\text{FeO}_{2.5}$ Using Site-resolved Energy-loss Near-edge Structures

Oxygen K-edge and Fe $L_{2,3}$ -edge electron energy-loss near-edge structures (ELNES) were measured for FeO_6 octahedra and FeO_4 tetrahedra in the brownmillerite $\text{Ca}(\text{Sr})\text{FeO}_{2.5}$ by focusing an electron probe at individual Fe sites using scanning transmission electron microscopy (STEM) combined with electron energy-loss spectroscopy (EELS). The observed site-resolved oxygen K-ELNES showed different features reflecting the local chemical bonding around the FeO_6 octahedra and FeO_4 tetrahedra. A pre-peak in the O K-edge spectra, which is attributed to a transition to an unoccupied O 2p band hybridized with the Fe 3d band, shows splitting in the spectrum of the FeO_6 octahedral site. Additionally, for the oxygen linking the octahedral and tetrahedral Fe sites in $\text{CaFeO}_{2.5}$, charge transfer was found to preferentially occur toward the tetrahedral Fe ions. In the case of $\text{SrFeO}_{2.5}$, charge transfer from the oxygen located in the *ac* plane was biased toward the tetrahedral Fe atoms. Based upon an analysis of the pre-peak intensity of the O K-ELNES, it was concluded that bonding between the oxygen and iron atoms at the tetrahedral site was more covalent in character than at the octahedral site. The strong covalent character of the tetrahedral sites would be one of the reasons for distortion in the FeO_6 octahedra in $\text{Ca}(\text{Sr})\text{FeO}_{2.5}$, as exhibited by an extension along the *b*-axis.

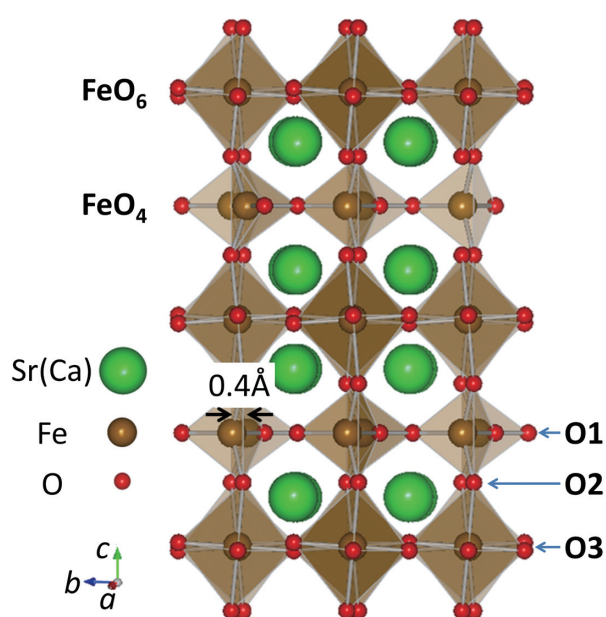


Figure 1. Structure model of brownmillerite $\text{Ca}(\text{Sr})\text{FeO}_{2.5}$. There are three nonequivalent oxygen atoms (O1, O2, and O3) in the unit cell.

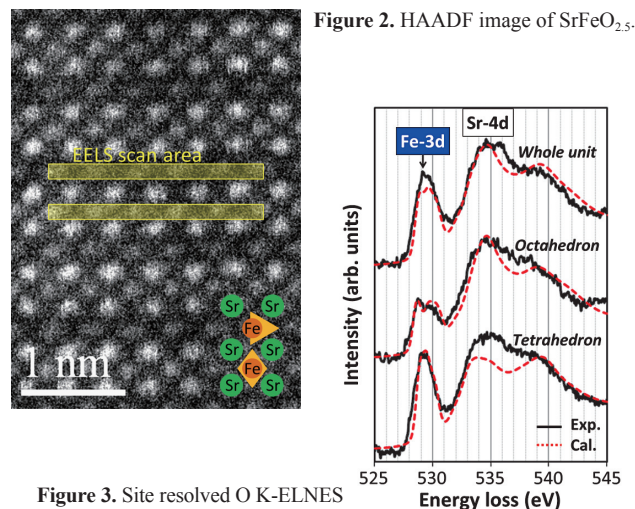


Figure 3. Site resolved O K-ELNES of $\text{SrFeO}_{2.5}$.

Interface Structure of Gold Particles on TiO_2 Anatase

Gold particles supported on titanium dioxide (TiO_2) are known to activate many catalytic reactions. In this study, interface structure of gold on anatase was examined in the case on an anatase $\{101\}$ surface, since the surface is the most important for several photocatalytic reactions. Anatase TiO_2 nanorods having clear washboard-like $\{101\}$ outer surfaces were synthesized by using a double surfactants system. From high resolution electron microscopy observation for gold particle on the $\{101\}$ surface, the (113) plane of gold was found to be parallel to the (101) surface of TiO_2 . Such an epitaxy is corresponding to be the axial and planar orientations of $[03\text{-}1] (200)\text{Au} // [-31\text{-}1] (113)\text{TiO}_2$, being originated from the smallest lattice mismatching, instead of the previous cases of $[01\text{-}1] (111)\text{Au} // [02\text{-}1] (112)\text{TiO}_2$ on the $\{110\}$ and $\{112\}$ surfaces of anatase TiO_2 .

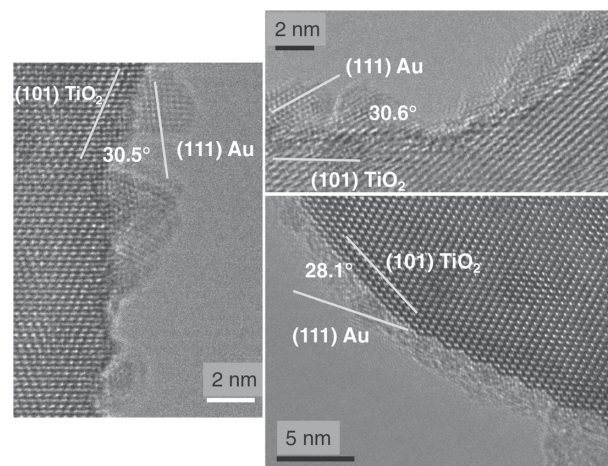


Figure 4. HR-TEM images of Au particles on $\{101\}$ surfaces of anatase TiO_2 nanorods.

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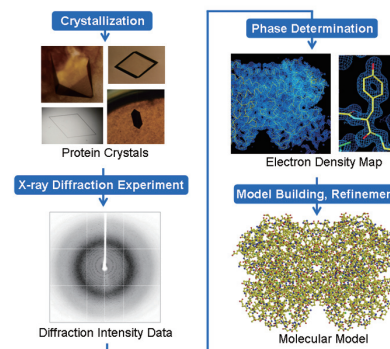
HOSOMI, Taku (M2)

Scope of Research

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

KEYWORDS

Crystal
X-ray Crystallographic Analysis
Racemase
Thermostability
D-Amino Acid



Selected Publications

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

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

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

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

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

Crystallographic Structure Analysis of Aspartate Racemase from *Lactobacillus sakei* NBRC-15893

Amino-acid racemases are responsible for the racemization of amino acids and can be mainly grouped into two families, pyridoxal 5'-phosphate (PLP) dependent and PLP independent. Aspartate racemase catalyzes the inter-conversion 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. Only the crystal structure of aspartate racemase from a hyperthermophilic archaeon has been reported so far. To elucidate the structure-function relationship of aspartate racemase which works in the range of the low to medium temperature, we have determined the crystal structure of aspartate racemase from *Lactobacillus sakei* NBRC-15893 (LsAspR).

Initial crystallization experiments were performed by the sitting-drop vapour-diffusion method using Crystal Screen I, Crystal Screen II, and PEGRx. Small crystals were obtained after several days with solution PEGRx #58. The crystallization conditions were optimized based on those of the solution. The final conditions produced rod-shaped crystals with approximate dimensions of $0.4 \times 0.15 \times 0.03$ mm at 293 K in 3 days using the sitting-drop vapour-diffusion method with seeding technique (Figure 1). Drops of 1 μ l protein solution at 20 mg/ml (in 50 mM MES buffer, pH 6.5, 4 mM dithiothreitol) and 1 μ l reservoir solution were equilibrated against 100 μ l reservoir solution consisting of 25% (v/v) PEG-MME 550, 5% (v/v) 2-Propanol, and 0.1 M Sodium acetate, pH 4.8.

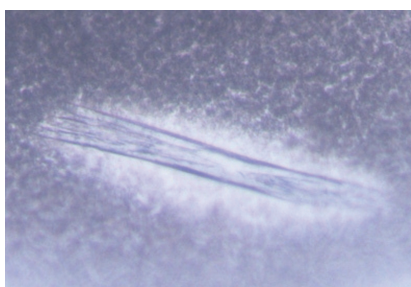


Figure 1. Crystal of aspartate racemase from *Lactobacillus sakei* strain NBRC-15893.

Diffraction experiments were performed at beamline NE-3A, Photon Factory AR, Tsukuba, Japan. The crystal was flash-cooled in a nitrogen stream at 100 K. Diffraction data were collected at a wavelength of 1.000 Å using a Quantum 270 CCD detector set to 331.2 mm in a crystal-

to-detector distance. The crystals belonged to space group $P3_121$ with unit cell parameters of $a=b=105.5$ Å and $c=96.5$ Å. The data set was collected at 2.6 Å resolution and has 20,826 independent reflections with completeness of 99.7%. The asymmetric unit contained one dimeric molecule of LsAspR with a corresponding crystal volume per protein mass (V_M) of 2.97 Å³/Da and a solvent content of 59%. The crystal structure has been determined by molecular replacement. The current model was refined at 2.6 Å resolution to an R -factor of 23.8% ($R_{\text{free}}=31.6\%$).

In crystals, LsAspR adopts a homodimeric form (Figure 2). The subunit consists of two domains: the N-terminal domain (residues 1–104 and 216–234) and the C-terminal domain (residues 105–215). In each domain, a central four-stranded parallel β -sheet is flanked by six α -helices. The spatial arrangement of the strictly conserved residues Cys84 and Cys196 strongly indicates that the active site of LsAspR must be located in the cleft between the two domains (Figure 3).

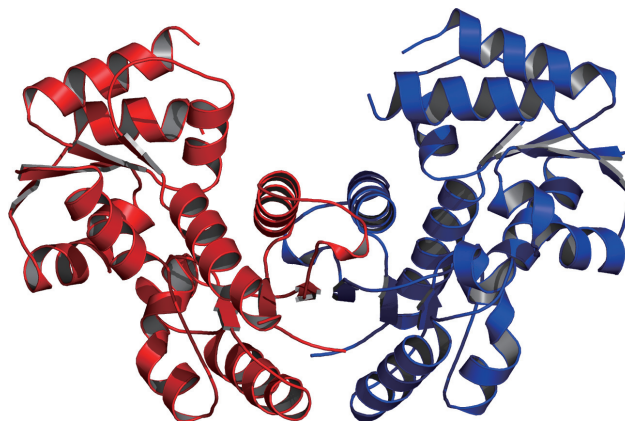


Figure 2. Dimeric molecular structure of aspartate racemase from *Lactobacillus sakei* strain NBRC-15893.

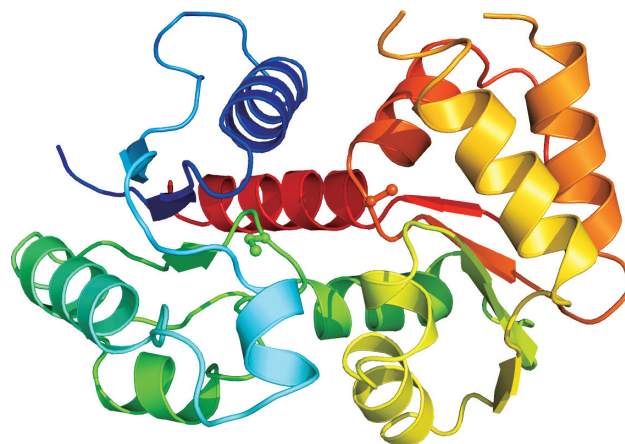


Figure 3. Subunit structure of aspartate racemase from *Lactobacillus sakei* strain NBRC-15893. The strictly conserved residues Cys84 and Cys196 are shown as ball-and-stick models.

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Visitor

Prof HOU, Xue-Long Shanghai Institute of Organic Chemistry, China, P.R., 10 March

Scope of Research

Our research activity is focused on the development of molecular transformation reactions, which can provide new ways to exploit chemical resources, such as haloalkanes, alkenes, alcohol etc. The present research subjects are (1) metal-catalyzed C–C bond forming reactions by using universal metals such as iron, magnesium and aluminum (2) development of smart materials based on synergistic effect of various metals on artificial peptide (3) synthesis of heteroatom-fused π -conjugated molecules toward optoelectronics (4) understanding of synergistic effects of multi-element center interactions for the catalysis with the help of quantum chemical methods and spectroscopy.

KEYWORDS

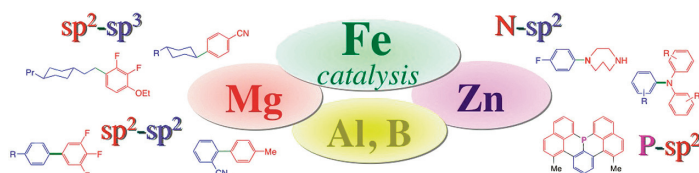
Carbon–Carbon Bond Formation

Iron Catalyst

Cross-Coupling Reaction

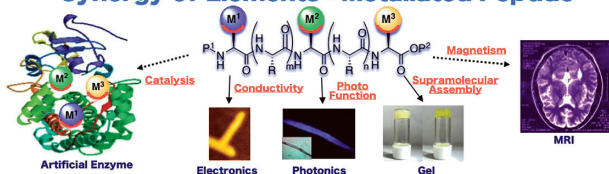
Metallated Peptide

π -Conjugated Molecule



Pursuit of Elements : Catalysis and Synthesis

Synergy of Elements : Metallated Peptide



Selected Publications

Hatakeyama, T.; Hashimoto, S.; Seki, S.; Nakamura, M., Synthesis of BN-fused Polycyclic Aromatics via Tandem Intramolecular Electrophilic Arene Borylation, *M. J. Am. Chem. Soc.*, **133**, 18614-18617 (2011).

Hatakeyama, T.; Okada, Y.; Yoshimoto, Y.; Nakamura, M., Tuning Chemoselectivity in Iron-Catalyzed Sonogashira-type Reaction Using a Diphosphine Ligand with Peripheral Steric Bulk: Selective Alkynylation of Non-activated Alkyl Halides, *Angew. Chem. Int. Ed.*, **50**, 10973-10976 (2011).

Ito, S.; Itoh, T.; Nakamura, M., Diastereoselective Carbometallation of Oxa- and Azabicyclic Alkenes under Iron Catalysis, *Angew. Chem. Int. Ed.*, **50**, 454-457 (2011).

Ishizuka, K.; Seike, H.; Hatakeyama, T.; Nakamura, M., Nickel-Catalyzed Alkenylative Cross-Coupling Reaction of Alkyl Sulfides, *J. Am. Chem. Soc.*, **132**, 13117-13119 (2010).

Hatakeyama, T.; Hashimoto, T.; Kondo, Y.; Fujiwara, Y.; Seike, H.; Takaya, H.; Tamada, Y.; Ono, T.; Nakamura, M., Iron-Catalyzed Suzuki-Miyaura Coupling of Alkyl Halides, *J. Am. Chem. Soc.*, **132**, 10674-10676 (2010).

Tuning Chemoselectivity in Iron-Catalyzed Sonogashira-type Reaction Using a Diphosphine Ligand with Peripheral Steric Bulk

A chemoselective Sonogashira-type coupling of primary and secondary alkyl halides with alkynyl Grignard reagents have been developed by using an iron catalyst. The key to success is the use of diphosphine ligand bearing peripheral steric bulk, which dramatically switches chemoselectivity from the C_{sp^2} -selective coupling to C_{sp^3} -selective coupling. The present reaction can be applicable to secondary alkyl halides, including less-reactive alkyl chlorides, which are difficult substrate with the previous methods. These synthetic advantages, as well as the non-hazardous nature of the catalyst and reagents make the present reaction suitable for facile synthesis or production of various functional molecules bearing alkyne moieties.

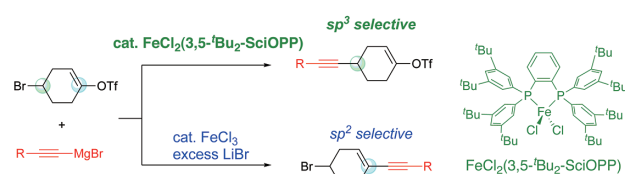


Figure 1. Chemoselective cross-coupling using a novel iron-diphosphine complex.

Programmable Metal Unit Arrangement on Peptides to Create Composition- and Configuration-Controlled Heterometallic Hybrid Materials

This project focuses on the following challenges: i) Development of fundamental methodology for creating composition- and configuration-controlled heterometallic hybrid molecules using metallated-amino acids and peptides as metal units. Chemical synthesis and self-assembly process of the metal units is currently employed, in complementary, to control the composition, 1D/2D array, and 3D configuration of metals on peptides i.e., programmable metal unit arrangements. ii) Exploring the function of heterometallic hybrid molecules. Applications to supra-molecular gelators, molecular electronic devices, photo-chemical devices, advanced catalysts, artificial enzymes, and MRI contrast agents are ongoing with a diverse library of metallated-amino acids and peptides.

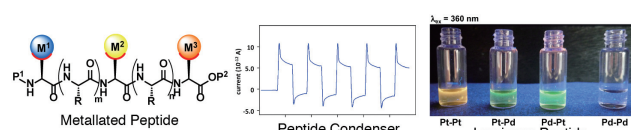


Figure 2. Preparation of metallated peptide and self-assembly of the peptide.

Synthesis of BN-fused Polycyclic Aromatics via Tandem Intramolecular Electrophilic Arene Borylation

A tandem intramolecular electrophilic arene borylation reaction has been developed for the synthesis of BN-fused polycyclic aromatic compounds such as 4b-aza-12b-boradibenzo[*g,p*]chrysene **A** ($n=0$) and 8b,11b-diaza-19b,22b-diborahexabenzo[*a,c,f,g,j,l,op*]tetracene **B** ($n=1$). These compounds adopt a twisted conformation, which results in a tight and offset face-to-face stacking array in the solid state. Time-resolved microwave conductivity measurements prove that the intrinsic hole mobility of **A** ($0.07 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) is comparable to that of rubrene ($0.05 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$), one of the most commonly used organic semiconductors, indicating that BN-substituted PAHs are potential candidates for organic electronic materials.

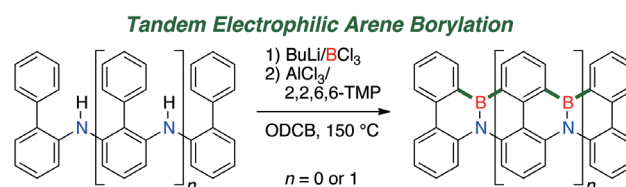


Figure 3. Synthesis of BN-fused polycyclic aromatics.



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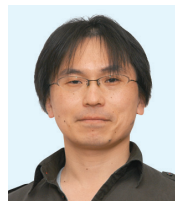
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SEKI, Hayato (M2)

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NISHI, Hitomi (M1)
YAMADA, Marina (M1)

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Prof Kennedy, Brendan School of Chemistry The University of Sydney, Australia, 10–22 July

Scope of Research

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

KEYWORDS

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



Selected Publications

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. Reports*, **1**, 27 (2011).
Azuma, M.; Chen, W. T.; Seki, H.; Czapski, M.; Olga, S.; Oka, K.; Mizumaki, M.; Watanuki, T.; Ishimatsu, N.; Kawamura, N.; Ishiwata, S.; Tucker, M. G.; Shimakawa, Y.; Attfield, J. P., Colossal Negative Thermal Expansion in BiNiO₃ Induced by Intermetallic Charge Transfer, *Nat. Comm.*, **2**, 347 (2011).
Inoue, S.; Kawai, M.; Ichikawa, N.; Kageyama, H.; Paulus, W.; Shimakawa, Y., Anisotropic Oxygen Diffusion at Low Temperature in Perovskite-Structure Iron Oxides, *Nat. Chem.*, **2**, 213-217 (2010).
Long, Y. W.; Hayashi, N.; Saito, T.; Azuma, M.; Muranaka, S.; Shimakawa, Y., Temperature-induced A-B Intersite Charge Transfer in an A-site-ordered LaCu₃Fe₄O₁₂ Perovskite, *Nature*, **458**, 60-63 (2009).
Kan, D.; Terashima, T.; Kannda, R.; Masuno, A.; Tanaka, K.; Chu, S.; Kan, H.; Ishizumi, A.; Kanemitsu, Y.; Shimakawa, Y.; Takano, M., Blue-light Emission at Room Temperature from Ar⁺-irradiated SrTiO₃, *Nat. Mater.*, **4**, 816-819 (2005).

Material Design and High-pressure Synthesis of Novel A-site-ordered Perovskites

A-site-ordered perovskite oxides with chemical formula $AA'_3B_4O_{12}$ have a rich variety of physical and chemical properties, such as intersite charge transfer. To further explore novel compounds with this A-site-ordered structure, we evaluated structural stability by calculating the global instability index (GII) with the SPuDS program and designed new compounds based on the calculation results. We especially focus on the compound with Mn^{3+} in the square-planar A' site, $A^{3+}Mn^{3+}_3Al^{3+}_4O_{12}$ because the square-planar coordination of the Mn^{3+} ion is very rare in oxide materials, and it is expected that such unique coordination would have unusual electronic structure and results in interesting magnetic properties. Also selecting the non magnetic Al^{3+} ion in B-site makes it easier to investigate how the square-planarly coordinated Mn^{3+} ion magnetically behaves.

From the structural stability of hypothetical $AMn_3Al_4O_{12}$ (A = lanthanoid ions or Y ions), we find that the ionic radius in the A-site ion r_A increases, GII first decreases and reaches a minimum for Dy of which r_A is 1.08 Å. With further increasing r_A , the GII increases. This suggests that with the A^{3+} ions having r_A near 1.08 Å, the $AMn_3Al_4O_{12}$ structure become most stable. Thus we selected Y, Yb, and Dy for the A-site elements.

With high-pressure synthesis technique we have succeeded in synthesizing those designed compounds with a cubic $Im-3$ $AA'_3B_4O_{12}$ perovskite structure.

Structural parameters obtained from the structure refinement well agreed with the "predicted" values. Magnetic property measurements revealed that the Mn^{3+} ions at the square-planar A-site provides $S = 2$ spins, which are antiferromagnetically ordered at temperatures ranging from 29 to 40 K due to the direct exchange interaction. It is also found that the moment of Yb^{3+} and Dy^{3+} ion showed paramagnetic behaviors even below the antiferromagnetic transition temperatures.

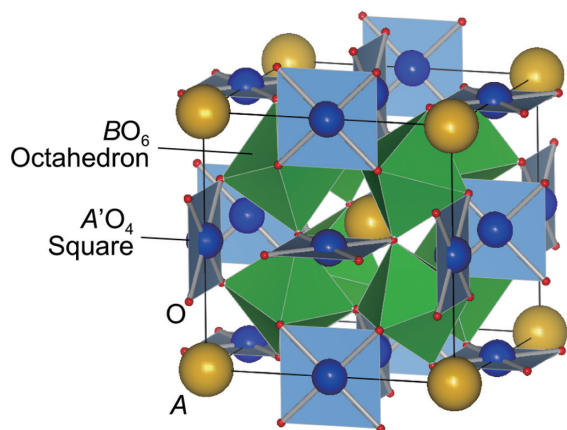


Figure 1. Crystal structure of A-site-ordered perovskite $AA'_3B_4O_{12}$.

Selective Reduction of Layers at Low Temperature in Artificial Superlattice Thin Films

Oxygen-deficient perovskites $AFeO_{3-\delta}$ ($A = Sr$ or Ca and $\delta = 0\sim 1.0$) attract much attention because they show wide varieties in crystal structures and physical properties as a function of oxygen content, and thus they have been studied extensively for more than 40 years. For example, $SrFeO_3$ ($\delta = 0$) is a simple perovskite, contains iron ions with unusually high valence state (Fe^{4+}), which is stabilized by a strong oxidizing atmosphere, and exhibits metallic conductivity. $SrFeO_{2.5}$ ($\delta = 0.5$), on the other hand, is synthesized at an ambient condition, and its brownmillerite structure consists of alternate layers of Fe^{3+} octahedra and tetrahedra, and is an antiferromagnetic insulator. It has been demonstrated that low-temperature topochemical reduction can make the brownmillerite $SrFeO_{2.5}$ to an infinite-layer structure $SrFeO_2$ ($\delta = 1.0$). Such a wide range of oxygen nonstoichiometry could also be exploited in applications for electrochemical energy generation and storage devices.

Recently we found the selective topochemical reduction occurs when artificial superlattices with transition-metal oxides are treated at a temperature below 300°C with CaH_2 . $[CaFeO_{2.5}]_m/[SrTiO_3]_n$ infinite-layer/perovskite artificial superlattice thin films were obtained by low-temperature reduction of $[CaFeO_{2.5}]_m/[SrTiO_3]_n$ brownmillerite/perovskite artificial superlattice thin films. By the reduction only the $CaFeO_{2.5}$ layers in the artificial superlattices were reduced to the $CaFeO_2$ infinite layers whereas the $SrTiO_3$ layers were unchanged. The observed low-temperature reduction behaviors strongly suggest that the oxygen ion diffusion in the artificial superlattices is confined within the two-dimensional brownmillerite layers and the stable $SrTiO_3$ layers can act as barriers for the oxygen diffusion. The reduced artificial superlattice could be reoxidized, and thus, the selective reduction and oxidation of the constituent layers in the perovskite-structure framework occur reversibly.

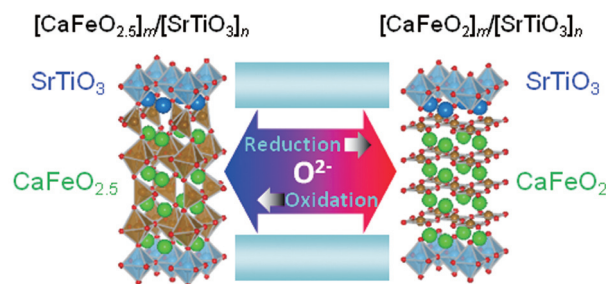


Figure 2. Reversible changes from $[CaFeO_{2.5}]_m/[SrTiO_3]_n$ to $[CaFeO_2]_m/[SrTiO_3]_n$ superlattice. The oxygen ion diffusion is confined within the two-dimensional brownmillerite layers.

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Scope of Research

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

KEYWORDS

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



Selected Publications

Takita, R.; Fujita, D.; Ozawa, F., Direct Arylation of Heteroarenes Catalyzed by a Pd/1,10-Phenanthroline Complex, *Synlett (Special Issue Dedicated to Professors Lixin Dai and Xiyun Lu)*, 959-963 (2011).

Nakajima, Y.; Shiraishi, Y.; Tsuchimoto, T.; Ozawa, F., Synthesis and Coordination Behavior of Cu^I Bis(phosphaethenyl)pyridine Complexes, *Chem. Commun.*, **47**, 6332-6334 (2011).

Okazaki, M.; Tsuchimoto, T.; Nakazawa, Y.; Takano, M.; Ozawa, F., Reaction of Bromoacetylene with Primary Amine on a Butterfly-Type Tetrairon Core to Give Isonitrile and Methyne through Oxidation and Deprotonation, *Organometallics*, **30**, 3487-3489 (2011).

Synthesis and Coordination Behavior of Cu(I) Bis(phosphaethenyl)pyridine Complexes

Phosphaalkenes with P=C bond(s) are low-coordinate phosphorus compounds, which possess extremely low-lying π^* orbitals around the phosphorus atom(s) and thus exhibit strong π -acceptor properties towards transition metals. In this study, we found that Cu(I) complexes bearing BPEP as a PNP-pincer type phosphaalkene ligand undergo effective bonding interactions with SbF_6^- and PF_6^- as non-coordinating anions to give $[\text{Cu}(\text{SbF}_6)(\text{BPEP})]$ (BPEP) and $[\text{Cu}_2(\text{BPEP})_2(\mu\text{-PF}_6)]^+$, respectively [BPEP = 2,6-bis(1-phenyl-2-phosphaethenyl)pyridine]. NMR and theoretical studies indicated a reduced anionic charge of the $\mu\text{-PF}_6$ ligand, which is induced by the strong π -accepting ability of BPEP.

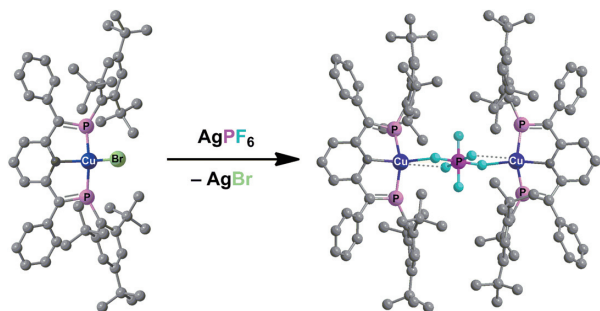


Figure 1. Formation of $[\text{Cu}_2(\text{BPEP})_2(\mu\text{-PF}_6)]^+[\text{PF}_6]^-$.

Redox Chemistry of Bis(phosphaethenyl)pyridine Iron Complexes

Redox chemistry of iron complexes has drawn increasing attention in connection with activation of small molecules in enzymatic systems. In this study, we investigated the redox properties of iron dibromide $[\text{FeBr}_2(\text{BPEP})]$ and iron monobromide $[\text{FeBr}(\text{BPEP})]$ coordinated with BPEP as a tridentate PNP-pincer type phosphaalkene ligand. Treatment of $[\text{FeBr}_2(\text{BPEP})]$ with $\text{Mes}_2\text{Mg}(\text{THF})_2$ (Mes = 2,4,6- $\text{Me}_3\text{C}_6\text{H}_2$) led to one-electron reduction to afford $[\text{FeBr}(\text{BPEP})]$, followed by transmetalation giving $[\text{FeMes}(\text{BPEP})]$ with a four-coordinate Fe(I) center (Figure 2). It is likely that the π -conjugation effect, which is derived from the $d\pi\text{-}p\pi$ interaction between the Fe(I) and BPEP ligand, is responsible for the easy reduction of $[\text{FeBr}_2(\text{BPEP})]$ to Fe(I) complexes.

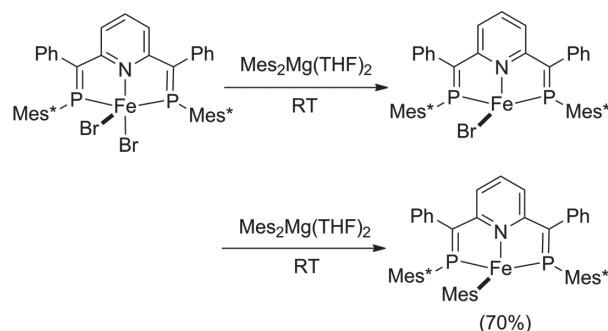


Figure 2. Reaction of $[\text{FeBr}_2(\text{BPEP})]$ with $\text{Mes}_2\text{Mg}(\text{THF})_2$.

Synthesis of End-capped Head-to-tail Regioregular Poly(3-hexylthiophene)s via Direct Arylation

While the catalytic dehydrohalogenative coupling of heteroarenes with aryl halides (so-called direct arylation) has received much attention in synthetic organic chemistry as an advanced means of C–C bond formation, its application to polycondensation has been poorly implemented until very recently. In this study, we have succeeded in the synthesis of head-to-tail regioregular poly(3-hexylthiophene)s end-capped with aryl groups (Ar-HT-P3HTs) using palladium-catalyzed polycondensation via direct arylation. As a typical example, heating a THF solution of 2-bromo-3-hexylthiophene (**1**), bromobenzene (1 equiv), $\text{Pd}\{o\text{-tolyl}\}_3$ (**2**, 2 mol%), **L** (2 mol%), Cs_2CO_3 (1 equiv), and KOAc (1 equiv) at 125°C for 36 h resulted in the formation of Ph-HT-P3HT with 99% regioregularity and M_n of 7100 in 99% yield, where 95% of the initiated end of polymer is capped with phenyl group as confirmed by ^1H NMR spectroscopy (Figure 3).

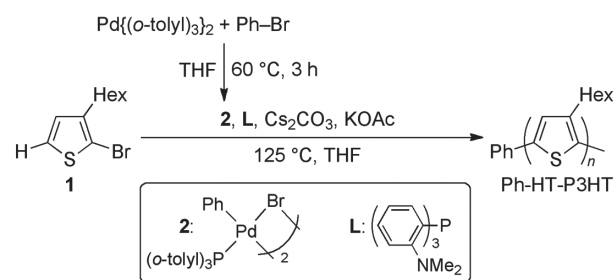


Figure 3. Synthesis of phenyl-capped HT-P3HT via direct arylation.

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KIMOTO, Yoshio (M1)

Scope of Research

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

KEYWORDS

Femtosecond Laser Spectroscopy
Carbon Nanotubes
Semiconductor Nanoparticles

Transition Metal Oxides
Semiconductor Nanostructures



Selected Publications

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

Yamada, Y.; Yasuda, H.; Tayagaki, T.; Kanemitsu, Y., Temperature Dependence of Photoluminescence Spectra of Undoped and Electron-doped SrTiO₃: Crossover from Auger Recombination to Single-carrier Trapping, *Phys. Rev. Lett.*, **102**, [247401-1]-[247401-4] (2009).

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

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

Observation of Charged Excitons in Hole-doped Carbon Nanotubes

Carbon nanotubes are one of the excellent materials for studying the optical properties of excitons, because of their unique band structures and large exciton binding energies. We report the first observation of trions (charged excitons), three-particle bound states consisting of one electron and two holes, in hole-doped carbon nanotubes at room temperature. When p-type dopants are added to carbon nanotube solutions, the photoluminescence and absorption peaks of the trions appear far below the E_{11} bright exciton peak, regardless of the dopant species. The unexpectedly large energy separation between the bright excitons and the trions is attributed to the strong electron-hole exchange interaction in carbon nanotubes.

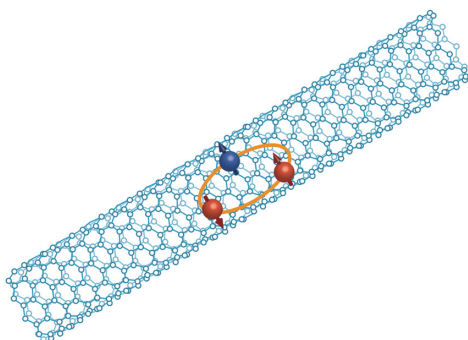


Figure 1. Schematic illustration of charged excitons in carbon nanotubes.

Quantized Auger Recombination of Biexcitons in CdSe Nanorods

Fabrication and characterization of semiconductor nanocrystals (NCs) have been extensively studied due to interest both in the fundamental physics and potential applications in optoelectronic devices. We studied the recombination dynamics of biexcitons in elongated CdSe nanocrystals (nanorods) using time-resolved photoluminescence (PL) and transient absorption (TA) spectroscopy. The decay times of the PL and TA signals decrease with increasing nanorod length. Under weak excitation, the PL decay is faster than the TA decay, and the nonradiative hole trapping determines the PL decay in several hundreds of picoseconds. Under intense excitation, the PL decay curves are similar to the TA decay curves, and the rapid biexciton decay is caused by nonradiative Auger recombination. A clear correlation is observed between the Auger recombination coefficient of the biexcitons and the average PL lifetime of the single excitons. Moreover, the Auger recombination lifetimes of the biexcitons are shorter in nanorods than in spherical nanocrystals of the same volume.

Our study clarified that the Auger recombination rate is strongly affected by a high surface-state density.

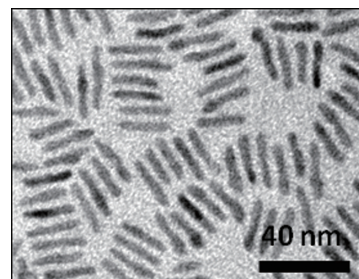


Figure 2. Transmission electron microscope image of elongated CdSe nanocrystals (nanorods).

High-Density Carrier Dynamics in Ge/Si Quantum Dots

Quantum dots (QDs) have attracted attention because of their interesting physical properties and potential applications in optoelectronic devices such as light emitters and solar cells. In QDs, physical processes of generation, relaxation, and recombination of carriers are determined by their nanostructures and differ from those in bulk crystals. We studied photoluminescence (PL) dynamics in thermally annealed Ge QDs in silicon crystals to determine the role of Ge-Si intermixing in carrier recombination processes. PL decay measurements revealed that the fast-decay component appeared under high-density photoexcitation, indicating nonradiative Auger recombination. By varying the annealing temperature of the QDs, the fast Auger decay time became larger than that of the as-grown QDs. This finding indicates that the Auger recombination rate is affected by Ge-Si intermixing due to thermal annealing.

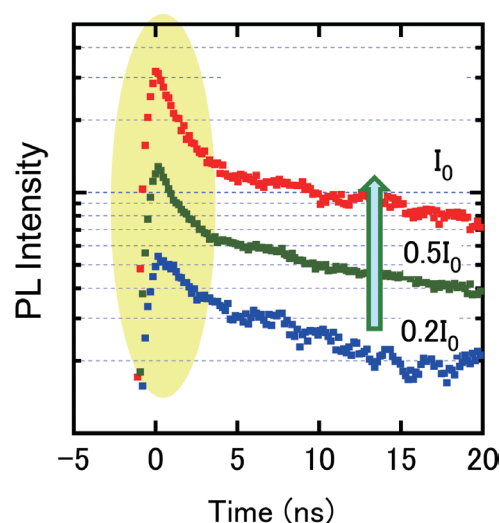


Figure 3. PL decay profiles at different photoexcitation intensities.

Bioinformatics Center – Chemical Life Science –

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



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Dr TSAI, Yu-Shuen National Yang-Ming University, Taiwan, 7 October 2011–30 April 2012

Scope of Research

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

KEYWORDS

KEGG
(Meta)genomics
Pathway
Bioinformatics
Metabolomics

Selected Publications

Takarabe, M.; Shigemizu, D.; Kotera, M.; Goto, S.; Kanehisa, M., Network-based Analysis and Characterization of Adverse Drug-drug Interactions, *J. Chem. Inf. Model.*, **51**, 2977-2985 (2011).
Kotera, M.; Tokimatsu, T.; Kanehisa, M.; Goto, S., MUCHA: Multiple Chemical Alignment Algorithm to Obtain Building Block Substructures of Orphan Metabolites, *BMC Bioinformatics*, **12(Suppl 14)**, S1 (2011).
Kirwan, G. M.; Diez, D.; Haeggstrom, J. Z.; Goto, S.; Wheelock, C. E., Systems Biology Approaches for Investigating the Relationships between Lipids and Cardiovascular Disease, *Curr. Cardiovasc. Risk Rep.*, **5**, 52-61 (2011).
Moriya, Y.; Shigemizu, D.; Hattori, M.; Tokimatsu, T.; Kotera, M.; Goto, S.; Kanehisa, M., PathPred: an Enzyme-catalyzed Metabolic Pathway Prediction Server, *Nucleic Acids Res.*, **38**, W138-W143 (2010).
Kanehisa, M.; Goto, S.; Furumichi, M.; Tanabe, M.; Hirakawa, M., KEGG for Representation and Analysis of Molecular Networks Involving Diseases and Drugs, *Nucleic Acids Res.*, **38**, D355-D360 (2010).



KEGG MEDICUS for Translational Bioinformatics

KEGG MEDICUS is a new resource for diseases, drugs and environmental substances, aiming to bring the genomic revolution to society. In KEGG, diseases are perturbed states in the molecular system and drugs are perturbants to the molecular system. Our knowledge on perturbed molecular system (network) is captured and presented as disease pathway maps in KEGG PATHWAY database. Other disease related knowledge on genetic and environmental perturbation is stored in KEGG DISEASE, listing known genetic factors (disease genes), environmental factors, diagnostic markers, and therapeutic drugs. All the marketed drugs in Japan, the OTC drugs as well as the prescription drugs, are fully represented in KEGG DRUG based on the chemical structures and/or the chemical components associated with target, metabolizing enzyme and other molecular network information. They are also integrated with the package insert information (labels information) that is applied to the adverse drug-drug interaction analysis described below. Health promoting and damaging substances such as crude drugs, essential oils, and other chemical substances are also collected and stored in KEGG ENVIRON with chemical component, efficacy and source species information whenever applicable. KEGG MEDICUS integrates the information in KEGG DISEASE, KEGG DRUG, KEGG ENVIRON, as well as other KEGG and outside databases in terms of genome-based biological systems (molecular network) information. As an attempt to integrate with outside resources, somatic mutation data obtained from Sanger Institute's COSMIC (Catalog Of Somatic Mutation In Cancer) database are mapped against KEGG cancer pathway and visualized in 3D map viewer (Figure 1).

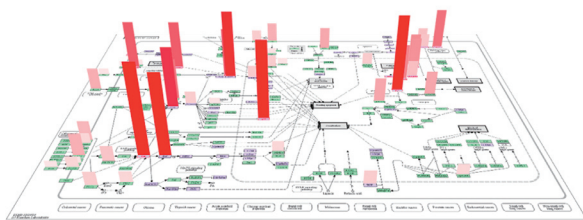
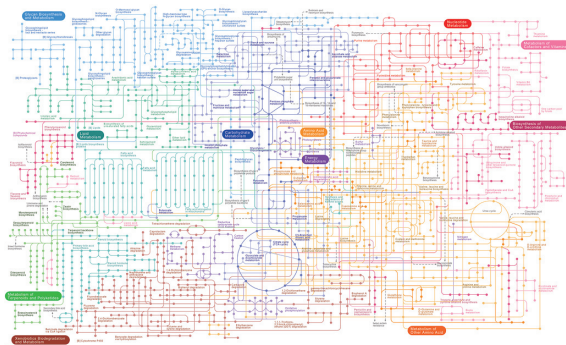


Figure 1. Cancer pathway map with somatic mutation frequency observed in colorectal cancer. The green boxes correspond to genes and the height or color-shading of the bar associated with each gene corresponds to the mutation frequency.



System Wide Analysis of Adverse Drug-drug Interactions

Co-administration of multiple drugs can cause adverse effects. It is becoming more important to provide a comprehensive view of drug-drug interactions among all the drugs in use, as well as a computational method to identify potential interactions. We extracted 1,306,565 known drug-drug interactions from all the package inserts of prescription drugs marketed in Japan. They were reduced to 45,180 interactions involving 1352 drugs (active ingredients) identified by the D numbers in the KEGG DRUG database, of which 14,441 interactions involving 735 drugs were linked to the same drug-metabolizing enzymes and/or overlapping drug targets. The interactions with shared targets were classified into three types: acting on the same target, acting on different but similar targets in the same protein family, and acting on different targets assigned to the same pathway. For the rest of the extracted interaction data, we attempted to characterize interaction patterns using drug group information. The drug groups were defined by the Anatomical Therapeutic Chemical (ATC) classification system, where the high-resolution network at the D number level is progressively reduced to a low-resolution global network. Based on this study we have developed a drug-drug interaction retrieval system in the KEGG DRUG database, which may be used for both searching against known drug-drug interactions and predicting potential interactions.

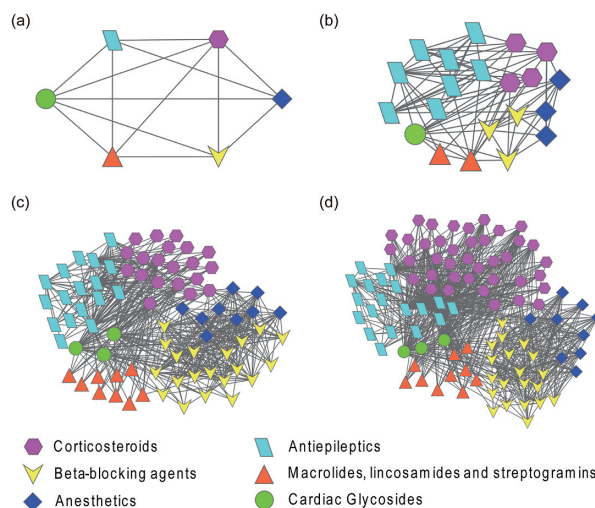


Figure 2. Drug interaction networks in the drug hierarchy.

Bioinformatics Center – Mathematical Bioinformatics –

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JIRA, Jindalertudomdee (M1)
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Visitors

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Assoc Prof CAPKOVIC, Frantisek

Prof ZHOU, Huarong

Dr SONG, Jiangning

Ben Gurion University, Israel, 8 March–5 June

Institute of Informatics Slovak Academy of Sciences, Slovenská republika, 2 June

Chinese Academy of Sciences, China, P.R., 13 September

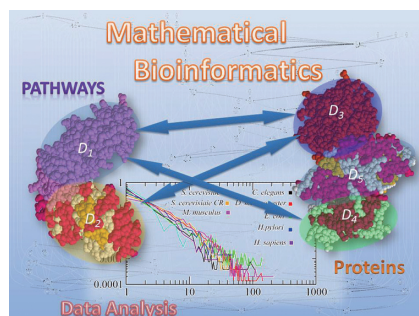
Monash University, Australia, 12 December 2011–27 January 2012

Scope of Research

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

KEYWORDS

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



Selected Publications

Akutsu, T.; Fukagawa, D.; Takasu, A.; Tamura, T., Exact Algorithms for Computing Tree Edit Distance between Unordered Trees, *Theoretical Computer Science*, **421**, 352-364 (2011).

Nacher, J. C.; Akutsu, T., On the Degree Distribution of Projected Networks Mapped from Bipartite Networks, *Physica A*, **390**, 4636-4651 (2011).

Imada, T.; Ota, S.; Nagamochi, H.; Akutsu, T., Efficient Enumeration of Stereoisomers of Outerplanar Chemical Graphs Using Dynamic Programming, *Journal of Chemical Information and Modeling*, **51**, 2788-2807 (2011).

Hayashida, M.; Kamada, M.; Song, J.; Akutsu, T., Conditional Random Field Approach to Prediction of Protein-Protein Interactions Using Domain Information, *BMC Systems Biology*, **5** (Suppl. 1), S8 (2011).

Sato, K.; Kato, Y.; Hamada, M.; Akutsu, T.; Asai, K., IPknot: Fast and Accurate Prediction of RNA Secondary Structures with Pseudoknots Using Integer Programming, *Bioinformatics*, **27**, i85-i93 (2011).

Discriminative Random Field Approach to Prediction of Protein Residue Contacts

For understanding constructions and evolution of biomolecular networks and cellular systems, it is important to analyze molecular recognition and specific interactions of proteins. Many investigations have been conducted to analyze interactions and contacts between residues. It is supported that residues at interacting sites have co-evolved with those at the corresponding residues in the partner protein to keep the interactions between the proteins. Therefore, mutual information (MI) between residues calculated from multiple sequence alignments of homologous proteins is considered to be useful for identifying contact residues in interacting proteins.

In our previous work, we proposed a prediction method for protein-protein interactions using mutual information and conditional random fields (CRFs), and confirmed its usefulness. The discriminative random field (DRF) is a special type of CRFs, and can recognize some specific characteristic regions in an image. Since the matrix consisted of mutual information between residues in two interacting proteins can be regarded as an image, we propose a prediction method for protein residue contacts using DRF models with mutual information. To validate our method, we perform computational experiments for several interactions between Pfam domains. The results suggest that the proposed DRF-based method with MI is useful for predicting protein residue contacts compared with that using the corresponding Markov random field (MRF) model.

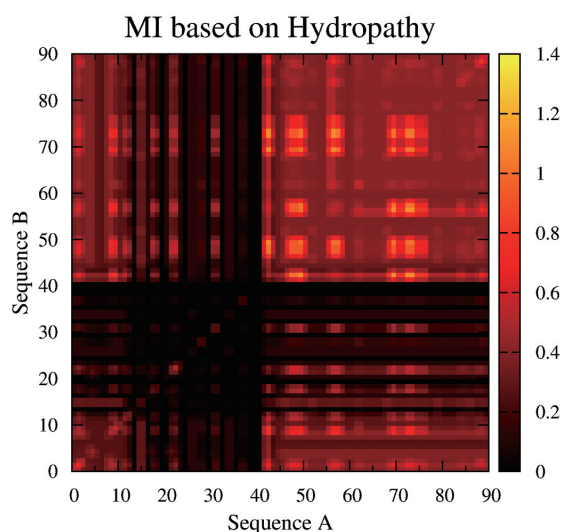


Figure 1. Mutual information between residues.

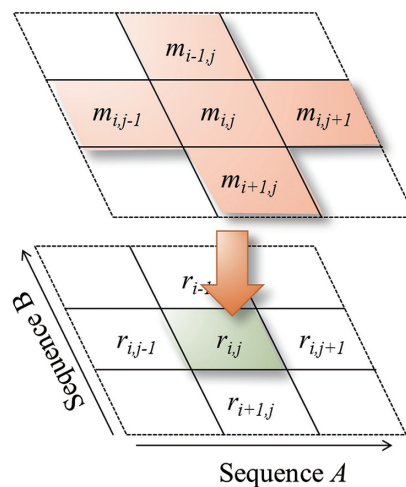


Figure 2. Discriminative random field model for protein residue interactions.

Computing Impact Degrees for Multiple Reactions in Metabolic Networks with Cycles

The impact degree is a measure of the robustness of a metabolic network against deletion of single or multiple reaction(s). Although such a measure is useful for mining important enzymes/genes, it was defined only for networks without cycles. In this work, we extend the impact degree for metabolic networks containing cycles and develop a simple algorithm to calculate the impact degree. Furthermore we improve this algorithm to reduce computation time for the impact degree by deletions of multiple reactions. We applied our method to the metabolic network of *E. coli*, that includes reference pathways, consisting of 3281 reaction nodes and 2444 compound nodes, downloaded from KEGG database, and calculate the distribution of the impact degree. The results of our computational experiments show that the improved algorithm is 18.4 times faster than the simple algorithm for deletion of reaction-pairs and 11.4 times faster for deletion of reaction-triplets. We also enumerate genes with high impact degrees for single and multiple reaction deletions.

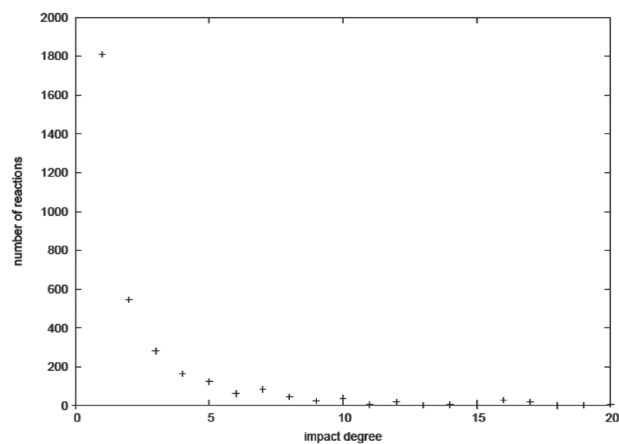


Figure 3. Distribution of impact degree for single-reaction deletion. The average impact degree is 2.651. The maximum impact degree is 55.

Bioinformatics Center – Bio-knowledge Engineering –

<http://www.bic.kyoto-u.ac.jp/pathway/>



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CHEN, Zhuoxin (RS)

Visitors

Assoc Prof ZHU, Shanfeng	Fudan University, China, P.R., 23 June–1 July
Assoc Prof KIHARA, Daisuke	Purdue University, U.S.A., 29 August
Assoc Prof WANG, Fang	Southwest University of China, China, P.R., 19 September 2011–31 March 2012
Prof FRISHMAN, Dmitrij	Technische Universitat Munich, Germany, 11 October
Prof VARNEK, Alexandre	University of Strasbourg, France, 18 November

Scope of Research

We are interested in graphs and networks in biology and chemistry, which include metabolic networks, protein-protein interactions and chemical compounds. We have developed original techniques in machine learning and data mining for analyzing these graphs and networks, sometimes combining with table-format datasets, such as gene expression. We applied our techniques to real data to find new scientific insights. You can see our Research Topics regarding more detailed contents of our achieved or ongoing research.

KEYWORDS

Bioinformatics
Computational Genomics
Data Mining
Machine Learning
Systems Biology

Selected Publications

Nguyen, C. H.; Mamitsuka, H., Discriminative Graph Embedding for Label Propagation, *IEEE Transactions on Neural Networks*, **22(9)**, 1395-1405 (2011).
Kayano, M.; Takigawa, I.; Shiga, M.; Tsuda, K.; Mamitsuka, H., ROS-DET: Robust Detector of Switching Mechanisms in Gene Expression, *Nucleic Acids Research*, **39(11)**, e74 (2011).
Takigawa, I.; Tsuda, K.; Mamitsuka, H., Mining Significant Substructure Pairs for Interpreting Polypharmacology in Drug-target Network, *PLoS One*, **6(2)**, e16999 (2011).
Shiga, M.; Takigawa, I.; Mamitsuka, H., A Spectral Approach to Clustering Numerical Vectors as Nodes in a Network, *Pattern Recognition*, **44(2)**, 236-251 (2011).
Takigawa, I.; Mamitsuka, H., Efficiently Mining d-Tolerance Closed Frequent Subgraphs, *Machine Learning*, **82(2)**, 95-121 (2011).

Latent Feature Models for Biological Networks

It is common in Systems Biology to represent biological systems as networks. Examples include the networks of protein-protein interactions (PPI) and gene regulatory networks (GRN). Biological networks, like many other types of networks, are known not to be random. Instead, network structures have models and patterns. By understanding the patterns and models of network structures, we would have insights into the biological mechanisms that generate the networks, leading to understanding of the generating processes of the networks. In the end, we would be able to infer knowledge of the biological systems, making judgments on what is on what is missing, what is erroneous. The understanding is to speed up experiment process by suggesting only relevant experiments to validate the understanding.

In this work, we aim to construct statistical models that describe network structures of PPI and GRN networks in order to *predict new links* (edges) in the networks. The motivation is that, for the case of physical protein-protein interactions, the binding site of each protein has to complement that of the other protein in shape. We hypothesize that the network structures follow *latent feature models*. The proof is that a link in the network is generated by a certain features of the nodes. These features alone determine the network structure around the nodes. By knowing all the features for the whole network, we would be able

to generate the complete network. What we need is just to generate these latent features to fit the currently known networks obtained from high-throughput experiments. However, the methods for generating the features to describe the networks are usually computationally intractable.

We propose to use nonparametric models to describe network structures that follow latent feature models. Instead of generating latent feature explicitly, we encode them implicitly by providing a similarity function (kernel) on the nodes of the networks. The method is described as in Figure 1. The input of the method is a network as in (1), we use its adjacency matrix (2) to compute the similarity function. With the assumption of latent feature model (4), we embed pairs of network nodes (either known links or not links (5)) into a space (3). In the space, we use usual classification techniques to classify the link class versus the rest. The half-space inferred from classifiers for the link class is used to predict all the pairs of nodes to make a new adjacency matrix (6). The new adjacency matrix is used for the predicted network (7), showing the new links as well as the erroneous ones.

We apply the method to predict new links in the networks of PPI (yeast and fruit fly) and GRN (*E. Coli*). Our method was able to run on the whole networks within minutes (while other methods do not stop for days). Our method gives high prediction scores on these networks, making our method a reliable and scalable one to predict new links on these biological networks.

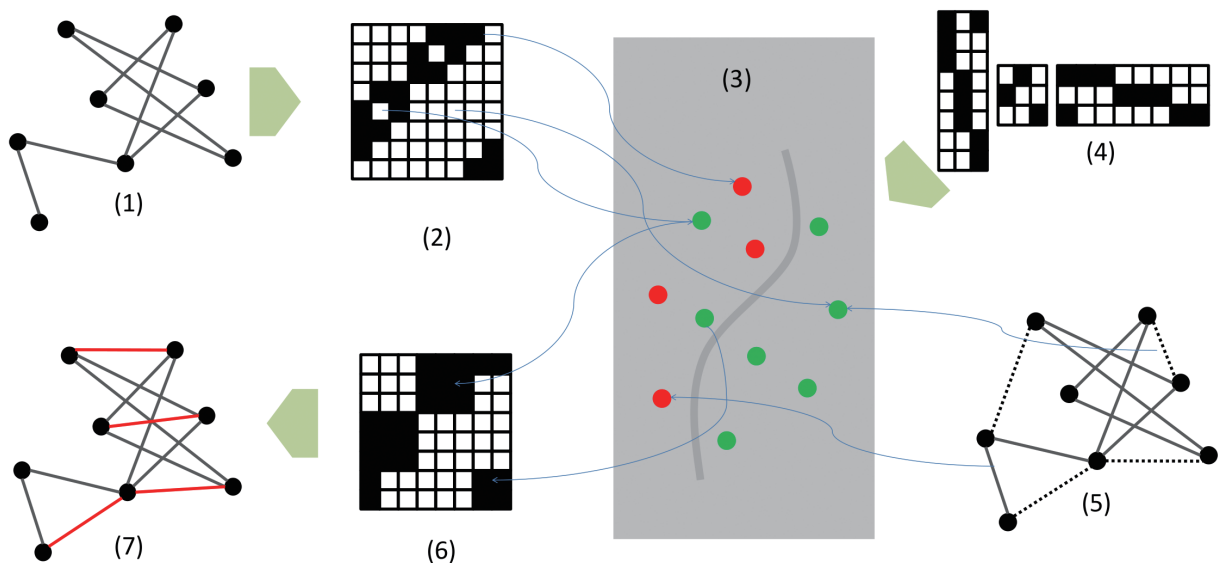


Figure 1.

Endowed Research Section – Water Chemistry Energy (AGC) –

<http://www.scl.kyoto-u.ac.jp/~nakahara/>



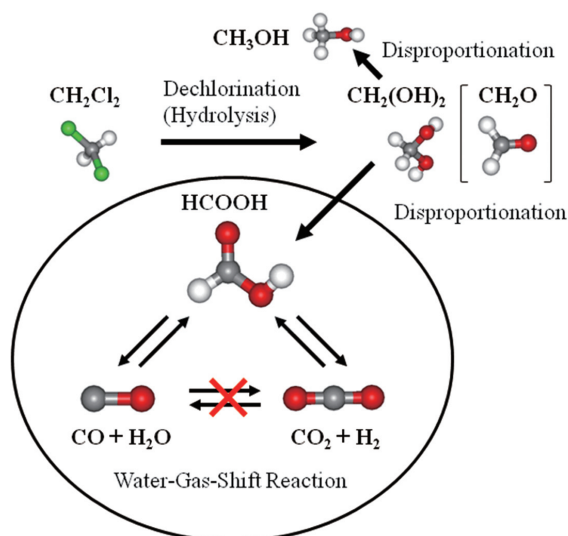
Vis Prof
NAKAHARA, Masaru
(D Sc)



Program-Specific Assist Prof
TSUJINO, Yasuo

Scope of Research

A novel energy system using formic acid has been put forward as a method for developing low-carbon hydrogen society. Kinetic, thermodynamic, and statistical mechanical principles of physical chemistry have been successfully applied for synthesizing formic acid from CO_2 and H_2 in near-room-temperature water without catalyst. To make public the achievement of our endowed research section we organized Kyoto Symposium on Novel Energy Systems. New mechanisms have been found for ether pyrolysis leading to renewable fuel molecules.



KEYWORDS

Formic Acid
Hydrogen
Carbon Dioxide
Water-Gas Shift Reaction
Carbon Neutral

Selected Publications

- Yasaka, Y.; Yoshida, K.; Wakai, C.; Matubayasi, N.; Nakahara, M., Kinetics and Equilibrium Study on the Formic Acid Decomposition in Relation to the Water-Gas-Shift Reaction, *J. Phys. Chem. A*, **110**, 11082-11090 (2006).
- Yasaka, Y.; Wakai, C.; Matubayasi, N.; Nakahara, M., Controlling the Equilibrium of Formic Acid with Hydrogen and Carbon Dioxide Using Ionic Liquid, *J. Phys. Chem. A*, **114**, 3510-3515 (2010).
- Yasaka, Y.; Klein, M. L.; Nakahara, M.; Matubayasi, N., Exploring the Reorientation of Benzene in an Ionic Liquid via Molecular Dynamics: Effect of Temperature and Solvent Effective Charge on the Slow Dynamics, *J. Chem. Phys.*, **134**, 191101-191104 (2011).
- Kimura, H.; Nakahara, M.; Matubayasi, N., In Situ Kinetic Study on Hydrothermal Transformation of D-Glucose into 5-Hydroxymethylfurfural through D-Fructose with ^{13}C NMR, *J. Phys. Chem. A*, **115**, 14013-14021 (2011).
- Tsujino, Y.; Yasaka, Y.; Matubayasi, N.; Nakahara, M., Pathways and Kinetics of Anisole Pyrolysis Studied by NMR and Selective ^{13}C Labeling. Heterolytic Carbon Monoxide Generation, *Bull. Chem. Soc. Jpn.*, **85**, 124-132 (2012).

Slow Reduction of Carbon Dioxide to Formic Acid Using Hydrogen in Ambient Water without Catalyst

Hydrogen comes from and returns to water of our environment when burned; $\text{H}_2 + 1/2\text{O}_2 = 1/2\text{H}_2\text{O}$. Hydrogen is thus renewable and clean. Hydrogen is obtainable from hot water via intermediate formic acid HCOOH as found in the new version of the Water-Gas-Shift reaction, $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{HCOOH} \rightleftharpoons \text{CO}_2 + \text{H}_2$. Hydrogen and oxygen in air are used for fuel cells to generate power without carbon dioxide emission. The burden on hydrogen society is the difficulty of hydrogen storage and transportation. Hydrogen gas has a low energy density, and it is often compressed into a bomb or liquefied at extremely low temperatures ($< -253^\circ\text{C}$) consuming energy. Hydrogen society needs a condensed matter, liquid that serves as a chemical tank for the reversible storage and release of hydrogen. Formic acid (liquid between 8.4 and 100.8°C) is such a candidate. A challenge is made here to develop a robust cycle reaction for hydrogen through formic acid. Carbon dioxide is slowly fixed as $\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{HCOOH}$. Principles of physical chemistry, kinetics and thermodynamics, are utilized here instead of metal catalysts em-

ployed in previous works. We are motivated to go back to the natural product water.

Water drives the fixation of carbon dioxide as formic acid when the reversibility is thermodynamically tuned. Water has a driving force due to the strong hydrogen-bonding hydration of formic acid on the product (HCOOH) side and the hydrophobic hydration of hydrogen on the reactant ($\text{CO}_2 + \text{H}_2$) side. Carbon dioxide is rather neutral between hydrophilicity and hydrophobicity; the equilibrium partition in the gas (hydrophobic) and water (hydrophilic) is neutral with the densities (concentrations) are almost the same in both phases. The yield reached in water at 70°C exceeds the previous one where catalyst and base are employed in supercritical carbon dioxide.

A high yield of formic acid has been realized as shown in Figure 1. The reaction temperature is lowered down to 80°C . The yield reaches >200 mM, which is the champion record compared to that obtained so far using rare metal catalysts. The water-driven synthesis of formic acid without catalyst is controlled not by the kinetics but by the thermodynamics. The lower the reaction temperature becomes, the higher the yield is. The yield enhancement by temperature lowering can be understood in view of the reaction exothermicity.

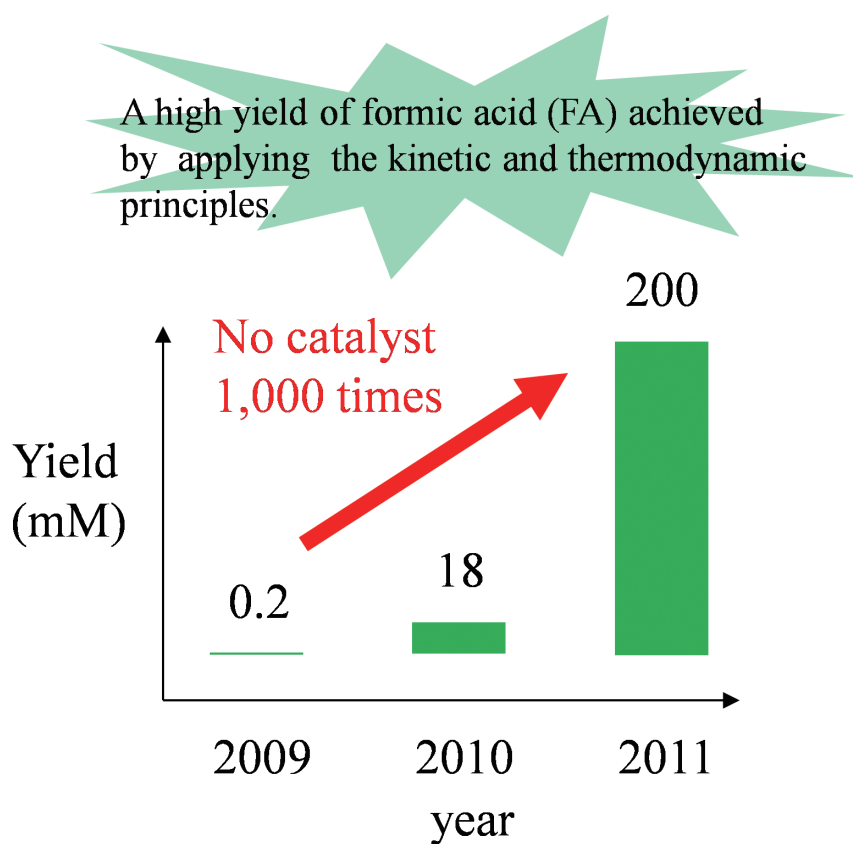


Figure 1. The hydrogen-water-energy-cycle via formic acid (FA) intermediate in the new version of the water-gas-shift reaction.

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

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



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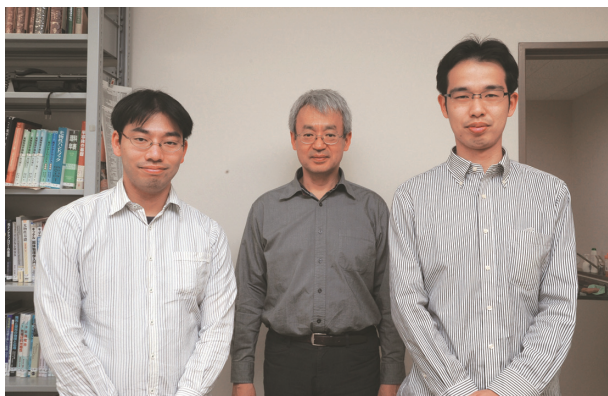
Prof (Supporting Faculty Member)
KANEMITSU, Yoshihiko
(D Eng)

Scope of Research

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

KEYWORDS

Nano-interface
Photovoltaic Science
Nanocarbon Materials
Transition Metal Oxides
Laser Spectroscopy
Solar Energy Conversion



Selected Publications

Okano, M.; Matsunaga, R.; Matsuda, K.; Masubuchi, S.; Machida, T.; Kanemitsu, Y., Raman Study on the Interlayer Interactions and the Band Structure of Bilayer Graphene Synthesized by Alcohol Chemical Vapor Deposition, *Appl. Phys. Lett.*, **99**, [151916-1]-[151916-3] (2011).

Yamada, Y.; Kanemitsu, Y., Blue Light Emission from Strongly Photoexcited and Electron-doped SrTiO₃, *J. Appl. Phys.*, **109**, [102410-1]-[102410-4] (2011).

Kanemitsu, Y.; Yamada, Y., Light Emission from SrTiO₃, *Phys. Stat. Sol. (b)*, **248**, 416-421 (2011).

Yamada, Y.; Kanemitsu, Y., Band-edge Luminescence from SrTiO₃: No Polaron Effect, *Thin Solid Films* (in press).

Yamada, Y.; Kanemitsu, Y., Photoluminescence Spectra of Perovskite Oxide Semiconductors, *J. Lumin.* (in press).

Nanointerface as a Platform to Develop Novel Optical Functionalities

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

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

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

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

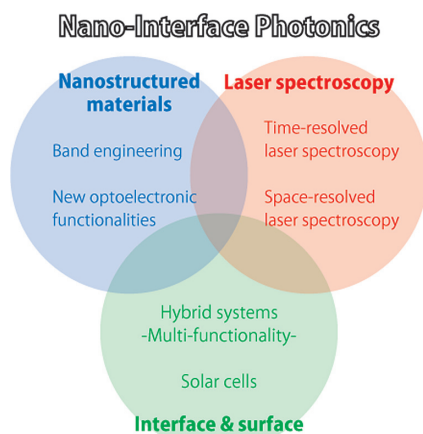


Figure 1.

Interlayer Interactions of Bilayer Graphene Studied by Raman Spectroscopy

Graphene has attracted interest because of its utility in fundamental physics research and potential device applications. We investigated the electronic band structure and interlayer interactions in graphene synthesized by alcohol-chemical vapor deposition (a-CVD) using microprobe Raman spectroscopy. The number of graphene layers was determined from the spectrally integrated intensity ratios of the *G* phonon to *2D* phonon peaks. We found that the value of the parameter determining interlayer interactions in a-CVD bilayer graphene was less than half that of exfoliated bilayer graphene. The weak interlayer interaction in a-CVD bilayer graphene was attributed to non-*AB* stacking order.

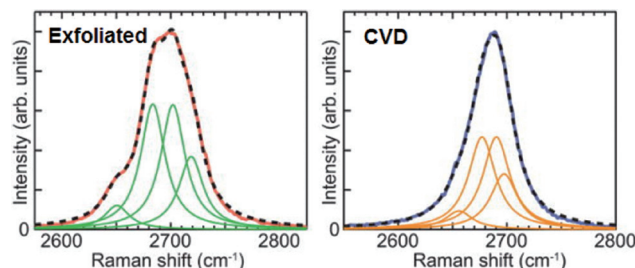


Figure 2. Raman spectra (thick solid curves), four Lorentzian components (thin solid curves), and fitting curves (dotted curves) of the *2D* phonon band in the exfoliated (left) and the a-CVD bilayer graphene (right) at 532-nm excitation.

Photoluminescence Properties and Carrier Characteristics of Perovskite Semiconductors

Perovskite oxides and their heterostructures have attracted a great deal of attention as new device materials because they show multifunctional properties beyond conventional semiconductors. However, their carrier dynamics still remain unclear. SrTiO₃ is a representative perovskite semiconductor, and we recently discovered band-edge photoluminescence (PL) at 3.2 eV in electron-doped or strongly photoexcited SrTiO₃ at low temperatures and assigned as band-to-band radiative recombination of free electrons and holes. On the other hand, other perovskite oxides, such as KTaO₃ and BaTiO₃ show no band-edge PLs but broad PL bands in the low-energy spectral region. These unique PL properties of SrTiO₃ are related to the high carrier mobility at low temperatures.



ACTIVITIES OF **J**OINT
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JURC Cooperative Research Subjects 2011

(1 April 2011 ~ 31 March 2012)

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

High-energy Ion Generation through the Interactions of Laser with Nano Particles

NAKAI, Mitsuo, Institute of Laser Engineering, Osaka University
Host in JURC TOKITA, Shigeki

Development and Application of Time-resolved Irradiation Method by Cooled Ion Beams

NODA, Koji, National Institute of Radiological Sciences
Host in JURC NODA, Akira

Optical and Electrical Properties of Mixed Organic Semiconductors

NAITO, Hiroyoshi, The School of Engineering, Osaka Prefecture University

Host in JURC KANEMITSU, Yoshihiko

Preparation of High-Performance Polycarbonate/Transition-Metal-Complex Hybrid Materials

KONISHI, Gen-ichi, Graduate School of Engineering, Tokyo Institute of Technology

Host in JURC OZAWA, Fumiyuki

Synthesis of Sugar-Acetylenes by Iron-Catalyzed Cross-Coupling and Study on Their Stimulus-Response Luminescence

ORITA, Masahiro, Faculty of Engineering, Okayama University of Science

Host in JURC NAKAMURA, Masaharu

Development of Negative Thermal Expansion Material Based on a Perovskite BiNiO_3

AZUMA, Masaki, Materials and Structures Laboratory, Tokyo Institute of Technology

Host in JURC SHIMAKAWA, Yuichi

Development of Novel 3-Dimensional π -Extended Molecules Directed toward Electronic Materials

SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University

Host in JURC MURATA, Yasujiro

Metagenome and Metatranscriptome Analysis of Soil Microbial Diversity and Functions in Natural and Degraded Tropical Rainforests

HARADA, Ko, Department of Forest Resources, Faculty of Agriculture, Ehime University

Host in JURC GOTO, Susumu

Integrated Analysis for Text Data and High Throughput Data Related to Metabolic Pathways

YONEZAWA, Akinori, Database Center for Life Science, Research Organization of Information and Systems

Host in JURC KANEHISA, Minoru

Efficient Search Algorithms for Structured Data in Bioinformatics

TAKASU, Atsuhiko, Digital Content and Media Sciences Research Division, National Institute of Informatics

Host in JURC AKUTSU, Tatsuya

Probabilistic Methods for Analysis on Protein Interaction Networks

MARUYAMA, Osamu, Institute of Mathematics for Industry, Kyushu University

Host in JURC AKUTSU, Tatsuya

Finding Frequent Similar Regions from Genome Sequences

NAKAMURA, Atsuyoshi, Graduate School of Information Science and Technology, Hokkaido University

Host in JURC MAMITSUKA, Hiroshi

Study of Functional Optical Thin Films by Sol-gel Method

IHARA, Rie, Department of Applied Physics, Tohoku University

Host in JURC MASAI, Hirokazu

Correlation of Structure and Electronic Structure in Thin Films of Group 10 Metals Dione-Dioximate

TAKEDA, Keiki, Graduate School of Engineering, Muroran Institute of Technology

Host in JURC SATO, Naoki

Structural Change of Frustrated Polymer Crystal at Low Temperature

OKIHARA, Takumi, Graduate School of Natural Science and Technology, Okayama University

Host in JURC TOSAKA, Masatoshi

Investigation of Extraction Behaviors of Metal Ions in Liquid-liquid Extraction Systems Using a Novel Multidentate Ligand

MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education

Host in JURC SOHRIN, Yoshiki

A New Soft-Interface Built of Stereocontrolled Hydrophilic Polymers

KATSUMOTO, Yukiteru, Graduate School of Science, Hiroshima University

Host in JURC HASEGAWA, Takeshi

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

X-Ray Structure Analysis of Reaction Mechanism of Catabolic Enzymes

OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University

Host in JURC HATA, Yasuo

X-Ray Structural Studies on Cold Adaptation of Proteins from Psychrophiles

GOUGAMI, Yoshitaka, Organization for Research and Development of Innovative Science and Technology, Kansai University

Host in JURC HATA, Yasuo

Multi-dimensional Doppler Laser Cooling for Realization of Ultralow-temperature Ion Beam

ITO, Kiyokazu, Graduate School of Advanced Sciences of Matter, Hiroshima University

Host in JURC NODA, Akira

Photocarrier Recombination Dynamics in Nanodomain-structured Ferroelectrics
FUNAKUBO, Hiroshi, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology
Host in JURC KANEMITSU, Yoshihiko

Design and Synthesis of Metal Ligands which Facilitate the Reductive Elimination Reaction and Their Application to the Synthesis of Cycloparaphenylenes
KORENAGA, Toshinobu, Graduate School of Natural Science and Technology, Okayama University
Host in JURC YAMAGO, Shigeru

Effective Transformation of Carbon-Resources on Dynamic Tetrairon Cores
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Development of Efficient Iron Catalysts for Selective Carbon-carbon Bond Forming Reactions Based on Mechanistic Studies
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC NAKAMURA, Masaharu

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

Efficient Construction of Polyfunctionalized Molecules by Cooperative Effect of Transition Metals and Heteroatoms
SEGI, Masahito, School of Chemistry, College of Science and Engineering, Kanazawa University
Host in JURC TOSHIMITSU, Akio

Prediction of Enzymatic Function of Cytochromes P450 Involved in Steroid Biosynthesis and Metabolism
OHNISHI, Toshiyuki, Division of Global Research Leaders, Shizuoka University
Host in JURC WATANABE, Bunta

Comprehensive Analysis of Calpain Substrate Specificity by the Integrated Data-mining Method
ONO, Yasuko, Tokyo Metropolitan Institute of Medical Science
Host in JURC MAMITSUKA, Hiroshi

Allele-specific Repertoire Overlap Analyzed by an HLA-binding Peptide Prediction Algorithm
UDAKA, Keiko, Kochi Medical School
Host in JURC MAMITSUKA, Hiroshi

Study on the Fabrication Process of Organic-inorganic Hybrid Materials
FUJINO, Shigeru, Department of Chemical Engineering, Faculty of Engineering, Kyusyu University
Host in JURC YOKO, Toshinobu

Cornea Regeneration by Small Molecule Fibronectin
KOIZUMI, Noriko, Faculty of Life and Medical Science, Doshisha University
Host in JURC UESUGI, Motonari

Development of a Technology for Solubilizing C₆₀ Fullerene Encapsulating an Atom(s) into Aqueous Solution
MURAKAMI, Masahiro, Department of Pharmacy, Osaka Ohtani University
Host in JURC MURATA, Yasujiro

Concentrated Polymer Brushes with Glucose-Sensing Ability
YOSHIKAWA, Chiaki, WPI-MANA, National Institute for Materials Science
Host in JURC TSUJII, Yoshinobu

Development of Novel Electrolyte for PEFC (Polymer Electrolyte Fuel Cell) by Living Radical Polymerization
MORINAGA, Takashi, Department of Chemistry Mechanical Engineering, Tsuruoka National College of Technology
Host in JURC TSUJII, Yoshinobu

Skin Permeation Using Arginine-rich Peptides
KOGURE, Kentaro, Kyoto Pharmaceutical University
Host in JURC FUTAKI, Shiroh

Time-resolved Grazing Incidence Small Angle X-ray Scattering for Dewetting in Polymer Blend Thin Films
OGAWA, Hiroki, Japan Synchrotron Radiation Institute
Host in JURC KANAYA, Toshiji

Studies on Crystal Structure and Formation Process of Poly(lactic acid)
KAWAI, Takahiko, Division of Production Science and Technology, Graduate School of Engineering, Gunma University
Host in JURC KANAYA, Toshiji

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

Electronic and Molecular Analysis of Biophysical and Biochemical Processes through Combined Quantum-Chemical/Statistical-Mechanical Approach
TAKAHASHI, Hideaki, Department of Chemistry, Graduate School of Science, Tohoku University
Host in JURC MATUBAYASI, Nobuyuki

Study of Dynamic Heterogeneity in Multi-Component Polymer Systems in Miscible State
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

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

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

Structure and Function of a Novel FADH₂-dependent Dehalogenase
KURATA, Atsushi, Department of Applied Biological Chemistry, Faculty of Agriculture, Kinki University
Host in JURC KURIHARA, Tatsuo

Preparation, Structure and Electronic Properties of Thin Films of Furan-Fused Polycyclic Aromatic Compounds
HAYASHI, Naoto, Graduate School of Science and Engineering for Research, University of Toyama
Host in JURC SATO, Naoki

Physics of THz Generation through the Interactions of Laser with Clusters
NAGASHIMA, Takeshi, Institute of Laser Engineering, Osaka University
Host in JURC HASHIDA, Masaki

Studies on Peculiar Changes in Higher-order Crystalline Lamellar Structures of Poly(ethylene glycol) upon Heating
SAKURAI, Shinichi, Biobased Materials Science, Graduate School of Science and Technology, Kyoto Institute of Technology
Host in JURC TOSAKA, Masatoshi

Development of Organic Solar Cell via the Interplay of Nanocarbon Science and Main Group Element Chemistry
TAJIMA, Tomoyuki, Graduate School of Environmental Science, Okayama University
Host in JURC TOKITOH, Norihiro

Domain Wall Oscillator by Spin Current
NAKATANI, Yoshinobu, Graduate School of Informatics and Engineering, University of Electro-Communications
Host in JURC ONO, Teruo

Study for Tunnel Magnetoresistive Effect and Local Magnetism of Magnetic Tunnel Junctions Using Co₂MnSn Heusler Alloy Electrodes Prepared by Atomically-controlled Alternate Deposition
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
Host in JURC ONO, Teruo

Small Molecules that Promote Differentiation into Pancreatic β Cells
KUME, Shouen, Institute of Molecular Embryology and Genetics, Kumamoto University
Host in JURC UESUGI, Motonari

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation
TOMINAGA, Rumi, Interdisciplinary Research Organization, University of Miyazaki
Host in JURC AOYAMA, Takashi

Overexpression of Miraculin Using *Arabidopsis thaliana*
INOUE, Hiroyasu, Faculty of Human Life and Environment
Host in JURC AOYAMA, Takashi

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

Search for New Method to Prepare Photovoltaic Device Using Reformed Coal Mixture
YAMASHITA, Makoto, Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University
Host in JURC MURATA, Yasujiro

Development of Supramolecular Multimetallic Catalyst for Selective Degradation of Lignins
WATANABE, Takashi, Research Institute for Sustainable Humanosphere, Kyoto University
Host in JURC NAKAMURA, Masaharu

Dynamics in the Interaction between Arginine-rich Peptides and Biomembranes
KOBAYASHI, Toshihide, ASI RIKEN
Host in JURC FUTAKI, Shiroh

Spin and Nuclear Spin Generation in Semiconductors by an Electrical Way
NITTA, Junsaku, Department of Materials Science, Tohoku University
Host in JURC KOBAYASHI, Kensuke

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Studies on the Transport and Metabolism of the Essential Trace Element Selenium in Mammals
MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
Host in JURC KURIHARA, Tatsuo

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

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

Development of Induction Systems in Plants Using Caged Chemicals
HAYASHI, Ken-ichiro, Department of Biochemistry, Okayama University of Science
Host in JURC AOYAMA, Takashi

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

Spectroscopic Study of the Influence of Gold on a Hierarchical Two-dimensional Molecular Aggregate of Supramolecules
YAMADA, Norihiro, Graduate School of Education, Chiba University
Host in JURC HASEGAWA, Takeshi

Dynamics in Physical Network Formed through Aggregation
SHIKATA, Toshiyuki, Graduate School of Science, Osaka University
Host in JURC MASUBUCHI, Yuichi

Development of Novel Electronic Phase Materials in Complex Iron-titanium Oxides
FUJII, Tatsuo, Faculty of Engineering, Okayama University
Host in JURC SAITO, Takashi

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Manipulation of π -conjugated Polymers by a Scanning Tunneling Microscope Tip
TAKAJO, Daisuke, Graduate School of Science, Osaka University
Host in JURC KURATA, Hiroki

Electron Spectroscopic Study of Degradation of Optical Properties
in First Mirror Materials for Fusion Plasma Diagnostics
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science
and Engineering, Shimane University
Host in JURC KURATA, Hiroki

NMR Characterization of Carbon Nitride
TAKARABE, Kenichi, Department of Applied Science, Okayama
University of Science
Host in JURC KAJI, Hironori

Solid-State NMR Analysis of Molecular Orientation in Organic
LED Materials
ADACHI, Chihaya, OPERA, Kyushu University
Host in JURC KAJI, Hironori

Solid-state-NMR Study on Luminescence and Structure Charac-
teristics of Organic Molecules
TOKUDOME, Yasuaki, Graduate School of Engineering, Osaka
Prefecture University
Host in JURC KAJI, Hironori

Systematic Syntheses and Properties of Polycyclic Aromatics
Containing a Phosphorus Atom
OKUMA, Kentaro, Department of Chemistry, Faculty of Science,
Fukuoka University
Host in JURC SASAMORI, Takahiro

Synthesis and Structure of Transition Metal Complexes with New
Tripodal Tetradentate Ligand
UNNO, Masafumi, Graduate School of Engineering, Gunma
University
Host in JURC TOKITOH, Norihiro

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

SUBJECTS ENCOURAGING JOINT PROGRAM

GEOTRACES JAPAN Symposium
GAMO, Toshitaka, Atmosphere and Ocean Research Institute,
The University of Tokyo
Host in JURC SOHRIN, Yoshiki

The 7th International Workshop for East Asian Young Rheologists
SAKURAI, Shinichi, The Center for Fiber and Textile Science,
Kyoto Institute of Technology
Host in JURC WATANABE, Hiroshi

Investigation on the Electronic States of Transition Metal Oxides
Containing Unusually High-valent Cations
KAWAKAMI, Takateru, Institute of Quantum Science, Nihon
University
Host in JURC SHIMAKAWA, Yuichi

JURC Publications

(until 31 May 2011)

A Clique-based Method for the Edit Distance between Unordered Trees and Its Application to Analysis of Glycan Structures

Fukagawa, D.; Tamura, T.; Takasu, A.; Tomita, E.; Akutsu, T., *BMC Bioinformatics*, **12**(Suppl 1), S13 (2011).

Abstract

This paper presents a practical method for computing the edit distance between rooted unordered trees. In this method, the original edit distance problem is transformed into the maximum clique problem and then efficient solvers for the maximum clique problem are applied. The proposed method was applied to similar structure search for glycan structures and the result suggests that the proposed method can efficiently compute the edit distance for moderate size unordered trees.

Algorithms for Finding a Minimum Repetition Representation of a String

Nakamura, A.; Saito, T.; Takigawa, I.; Mamitsuka, H.; Kudo, M., *LNCS 6393 (Proc. of SPIRE 2010)*, 185-190 (2010).

Abstract

A string with many repetitions can be written compactly by replacing h -fold contiguous repetitions of substring r with $(r)^h$. We refer to such a compact representation as a *repetition representation string* or RRS, by which a set of disjoint or nested tandem arrays can be compacted. In this paper, we study the problem of finding a *minimum RRS* or MRRS, where the size of an RRS is defined to be the sum of its component letter sizes and the sizes needed to describe the repetitions $(\bullet)^h$ which are defined as $w_R(h)$ using a repetition weight function w_R . We develop two dynamic programming algorithms to solve the problem. One is CMR that works for any repetition weight function, and the other is CMR-C that is faster but can be applied only when the repetition weight function is constant. CMR-C is an $O(w(n+z))$ -time algorithm using $O(n+z)$ space for a given string with length n , where w and z are the number of distinct primitive tandem repeats and the number of their occurrences, respectively. Since $w = O(n)$ and $z = O(n \log n)$ in the worst case, CMR-C is an $O(n^2 \log n)$ -time $O(n \log n)$ -space algorithm, which is faster than CMR by $((\log n)/n)$ -factor.

Enhanced Adsorption and Fluorescence Efficiency of Silylethynyl-functionalized Oligothiophenes and Thieno[3,2-*b*]thiophene

Asai, K.; Konishi, G.; Nakajima, Y.; Kawachi, S.; Ozawa, F.; Mizuno, K., *Journal of Organometallic Chemistry*, **696**, 1266-1271 (2011).

Abstract

We synthesized silylethynyl-substituted oligothiophenes and thieno[3,2-*b*]thiophenes by the palladium-catalyzed Sonogashira coupling reaction. These compounds exhibit longer absorbance and fluorescence peak wavelengths, higher absorption coefficients, and higher quantum efficiency than their corresponding unsubstituted molecules and *tert*-butylethynyl derivatives. From the DFT calculation, the energy band gap between HOMO and LUMO decreases by the introduction of a silicon atom. Thus, silyl groups can play important role in enhancing the quantum efficiency and decreasing the band-gap of chromophores. Hence, silylethynyl group can serve as a highly efficient auxiliary for use in optical devices.

Entanglement Dynamics in Miscible Polyisoprene/Poly(*p*-tert-butylstyrene) Blends

Watanabe, H.; Chen, Q.; Kawasaki, Y.; Matsumiya, Y.; Inoue T.; Urakawa, O., *Macromolecules*, **44**, 1570-1584 (2011).

Abstract

Viscoelastic, dielectric, and rheo-optical behavior was examined for miscible blends of high- M *cis*-polyisoprene (PI) and poly(*p*-*tert*-butylstyrene) (PtBS). The slow dielectric relaxation of the blends was exclusively attributed to the global motion of the PI chains having the type-A dipoles. The PI and PtBS chains behaved as the fast and slow (low- and high-friction) components and were well entangled with each other. The dynamics of these chains changed significantly with temperature T . At high T , the blend exhibited two-step entanglement plateau of the storage modulus $G'(\omega)$, and the plateaus at high and low angular frequencies (ω) were attributed, with the aid of the dielectric data, to the entanglement among all component chains and that between the PtBS chains, respectively. The entanglement length a characterizing the high- ω plateau was well described by a simple mixing rule based on the number fraction n of the Kuhn segments of the components, $a = n_{PI}a_{PI}^{bulk} + n_{PtBS}a_{PtBS}^{bulk}$. This result was consistent with the current molecular picture relating the entanglement density to the packing length p ($\approx a/20$). The complex moduli G^* of the blends in the high- ω plateau zone were well described by a simple blending law combined with this mixing rule of a , which was consistent with the rheo-optical data. At low T , the blend exhibited the Rouse-like power-law behavior of storage and loss moduli, $G' = G'' \propto \omega^{1/2}$, in the range of ω where the high- ω plateau was supposed to emerge. This lack of the high- ω plateau was attributed to retardation of the Rouse equilibration of the PI chain over the entanglement length a due to the hindrance from the slow PtBS chains: The PI and PtBS chains appeared to be equilibrated *cooperatively/simultaneously* at a rate essentially determined by PtBS. The Rouse equilibration time, evaluated from the G^* data of the blend, was just moderately shorter than the dielectrically determined relaxation time of PI. Thus, the high- ω plateau zone was too narrow to be resolved experimentally, and the PI chains relaxed almost immediately after their Rouse equilibration (retarded by PtBS). This PI relaxation activated the constraint release (CR) relaxation of PtBS to dilate the entanglement mesh for PtBS. A simple model considering the Rouse equilibration and CR/dilation processes described the G^* data of the blend surprisingly well, lending support to the molecular picture of the cooperative/simultaneous Rouse equilibration of the PI and PtBS chains. The model calculation was consistent with the rheo-optical data, which lent further support to this molecular picture.

Exact Algorithms for Computing the Tree Edit Distance between Unordered Trees

Akutsu, T.; Fukagawa, D.; Takasu, A.; Tamura, T., *Theoretical Computer Science*, **412**, 352-364 (2011).

Abstract

In this paper, we present a fixed-parameter algorithm for the edit distance problem for unordered trees under the unit cost model. The algorithm works in $O(2.62^k \cdot \text{poly}(n))$ time and $O(n^2)$ space, where the parameter k is the maximum bound of the edit distance and n is the maximum size of input trees. We also present polynomial time algorithms for the special case in which the maximum degree of the largest common subtree is bounded by a constant.



VISITING PROFESSORS'
ACTIVITIES IN ICR



Vis Prof
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Lecture at ICR

Syntheses, Structures, and Reactivity of
Low-valent Compounds of Heavier Main
Group Elements Stabilized by Alkyl
Substituents



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Lecture at ICR

Expression of Electronic Functions from
Nano-Radical Interfaces: Photo-Current
Convertors and Secondary Cells



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Lecture at ICR

Development of Ultrabroadband Terahertz
Time-Domain Spectroscopy and Its
Applications



Vis Prof
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Suwon, Gyeonggi-do 440-746, Korea, R.)



Vis Assoc Prof
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Lecture at ICR

Investigation of Liquid-Polymer Interface
by Coarse-Grained Modeling



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Lecture at ICR

Function of Lipids and Proteins in Bacterial
Membrane



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Lecture at ICR

Crystallographic Studies of Biological
Macromolecules with Synchrotron
Radiation



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Hokkaido 041-8655)

Lecture at ICR

Discoveries from Non-randomness in
Complex Cellular Networks and Systems



PERSONAL

Retirement

Professor KANEHISA, Minoru
Bioinformatics Center
– Chemical Life Science –



On March 31st 2012, Dr. Minoru Kanehisa retired from Kyoto University after 26 years of service and was honored with the title of Professor Emeritus of Kyoto University. Dr. Kanehisa was born in Nagasaki Prefecture on January 23rd 1948 and has dedicated his life to the noble pursuit of science and its dissemination. After receiving his PhD in physics in 1976 at the University of Tokyo under the supervision of Professor Akira Ikegami, Dr. Kanehisa travelled to the US, conducting post-doctoral research at Johns Hopkins University, Los Alamos National Laboratory, and the National Institutes of Health where he worked as a senior scientist. He was appointed an Associate Professor at the Institute for Chemical Research, Kyoto University in 1985 and promoted to Professor in 1987. In 2001 Dr. Kanehisa established the Bioinformatics Center in the Institute for Chemical Research, serving as its director until 2011. He has also held a position of adjunct Professor at the University of Tokyo (1991 to 1995, then again in 2002) and Boston University (2005).

Throughout his academic career, Dr. Kanehisa devoted himself to computational aspects of molecular and cellular biology; especially to the development of database and analysis systems for biologists and biochemists. While working at Los Alamos National Laboratory he was one of the core members responsible for initiating the GenBank database, a database of DNA sequences to which every researcher must submit new DNA sequences before publication.

Dr. Kanehisa also developed a database retrieval and analysis system called IDEAS (Integrated Database and Extended Analysis System for nucleic acids and protein). After starting his career at Kyoto University, Dr. Kanehisa established the GenomeNet database service by extending IDEAS to various molecular biology databases and computer platforms; its basic concept is still used in the current database services at GenomeNet.

In 1995, Dr. Kanehisa initiated the KEGG (Kyoto Encyclopedia of Genes and Genomes) project, one of the most important achievements of his academic career. KEGG is now widely used as a reference database by researchers from a variety of fields including omics, bioinformatics, systems biology, systems pharmacology, and

more. Together with GenomeNet, KEGG receives about 50 million accesses from 200,000 unique addresses per month.

Another contribution of Dr. Kanehisa to the institute was the introduction of a supercomputer system in 1991. It serves as a home for KEGG and GenomeNet services and developments and also provides chemical modeling applications for organic and inorganic chemists at Kyoto University. As of January 2012 its fifth update has been completed.

In addition to his own research interests, Dr. Kanehisa has served as a project leader for several national projects regarding bioinformatics research and education; *e.g.* the Genome Informatics Project supported by the Ministry of Education, Science, Sports and Culture during the very early stages of the human genome project (1991–2000), the 21st Century COE program for Genome Science (2003–2007), and the Education and Research Organization for Genome Information Science (2002–2006).

Dr. Kanehisa has provided his strong leadership to academic societies as well, especially within the bioinformatics community. Along with the initiation of the Genome Informatics Project in 1991, he initiated Genome Informatics Workshop (GIW), the world's oldest international conference on bioinformatics, renamed in 2001 to the International Conference on Genome Informatics due to the increasing number of annual participants. In 1999, he co-established the Japanese Society for Bioinformatics and served as its first chair.

Throughout his career Dr. Kanehisa's scientific achievements were published in over 200 original papers, some of them having been cited over 1,000 times. He was frequently invited to international conferences and collaborated with many foreign scientists from the USA, Germany, France, etc. He also contributed to various scientific meetings and international congresses as an executive committee member. He served as a member of the editorial board for many journals.

Dr. Kanehisa's contribution to Kyoto University and the Institute for Chemical Research is greatly acknowledged. His tireless scientific, educational and administrative endeavors will be appreciated for a long time to come.

Awards

SASAMORI, Takahiro



The Young Scientists' Prize of the Commendation for Science and Technology

“Creation of Novel π -Electron Systems of Heavier Group 14 Elements in Pursuit of Novel Function and Properties”

Ministry of Education, Culture, Sports, Science and Technology, Japan

11 April 2011

MURATA, Yasujiro



The Nozoe Memorial Award for Young Organic Chemists

The 22nd Symposium of Physical Organic Chemistry, Japan

“Studies on Structural Transformation of Fullerenes”

The Society of Physical Organic Chemistry, Japan

22 September 2011

KOBAYASHI, Kensuke



The 3rd Yukawa-Tomonaga Memorial Prize

“Experimental Study on the Electron Transport Based on Quantum Effect and Many-Body Effect in Semiconductor Devices”

Kyoto University

23 February 2011

The Young Scientists' Prize of the Commendation for Science and Technology

“Electron Transport based on Coherence and Many-body Effect in Semiconductors”

Ministry of Education, Culture, Sports, Science and Technology, Japan

11 April 2011

Funai Prize for Science

“Development of Semiconductor Devices Based on Quantum Many-body Effects and Their Dynamics”

The Funai Foundation for Information Technology

28 May 2011

CHIBA, Daichi



Ando Incentive Prize for the Study of Electronics

“Control of Magnetism by Electric Field”

The Foundation of ANDO Laboratory

18 June 2011

NAKASE, Ikuhiko



Young Investigator Award

“Mechanisms of Efficient Cellular Uptake of Arginine-Rich Cell-Penetrating Peptides”

The Japanese Peptide Society

28 September 2011

UESUGI, Motonari



The Pharmaceutical Society of Japan Award for Divisional Scientific Promotions 2011

“Control and Analysis of Cells by Synthetic Small Molecules”

The Pharmaceutical Society of Japan

28 March 2011

German Innovation Award Gottfried Wagener Prize (1st Prize)

“Development of Small Molecule Tools for Cell Therapy”

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

12 May 2011

SHINTANI, Megumi



Student Oral Presentation Award

Membrane Symposium 2011

“Intermolecular Interaction between Lipids and Small Molecules in Lipid Vesicles by Solution-State NMR-NOE and MD Simulation Study”

The Membrane Society of Japan

19 November 2011

MATSUMIYA, Yumi



The Encouraging Award of the Society of Rheology, Japan

“Fundamental Investigation of Polymer Dynamics with Dielectric and Viscoelastic Methods”

The Society of Rheology, Japan

19 May 2011

IMAI, Takeshi



Presentation Award

The 84th Annual Meeting of the Japanese Biochemical Society

“Studies of Selenite Reduction Pathway”

The Japanese Biochemical Society

24 September 2011

HATAKEYAMA, Takuji



Fluorine Chemistry Research Incentive Award

“Versatile Synthesis of Organofluorine Compounds Using Iron-Group-Metal Fluoride Catalysts”

Research Foundation ITSUU Laboratory

16 February 2011

INOUE, Rintaro



Award for Research Promotion

The 11th Annual Meeting of the Japanese Society for Neutron Science

“Dynamic Heterogeneity of Polymer Thin film as Studied by Neutron Scattering”

The Japanese Society for Neutron Science

22 November 2011

KAN, Daisuke



Young Scientist Oral Presentation Award

The 72nd Autumn Meeting of the Japan Society of Applied Physics

“Structural Transition in Epitaxial SrRuO₃ Thin Films”

The Japan Society of Applied Physics

30 August 2011

MASUBUCHI, Yuichi



The Encouraging Award of the 2nd Bridgestone Softmaterial Frontier Prize

“Simulation of Polymeric Networks”

The Society of Rubber Industry, Japan

30 May 2011

TAYAGAKI, Takeshi



The 5th Young Scientist Award

“Studies on the High-Density Photoexcited States in Semiconductor Materials”

The Physical Society of Japan

26 March 2011

MATSUNAGA, Ryusuke



President Prize of Kyoto University

“Spectroscopy in Carbon Nanotubes: Observation of Dark Excitons and Trions”

Kyoto University

11 March 2011

UEDA, Kei



The 22nd Award for Encouragement of Research in Condensed Matter Photophysics

“Dynamics of Quantized Auger Recombination in $\text{Si}_{1-x}\text{Ge}_x$ Nanocrystals”

20 December 2011

Paper Awards

MASAI, Hirokazu



JSAP Young Scientist Award

“High Photoluminescent Property of Low-Melting Sn-Doped Phosphate Glass”

Masai, H.; Takahashi, Y.; Fujiwara, T.; Matsumoto, S.; Yoko, T.

The Japan Society of Applied Physics

30 August 2011

FUTAKI, Shiroh, et. al.



2011 AAPS Journal Manuscript Award

“Delivery of Macromolecules Using Arginine-Rich Cell-Penetrating Peptides: Ways to Overcome Endosomal Entrapment”

Sayed, E. A.¹; Futaki, S.; Harashima, H.¹

American Association of Pharmaceutical Sciences

23 October 2011

¹ Graduate School of Pharmaceutical Sciences, Hokkaido University

NODA, Akira, et. al.



Original Paper Award of the Laser Society of Japan

“Ion Acceleration Using Temporally-Controlled High-Intensity Laser Pulses”

Yogo, A.; Daido, H.; Mori, M.; Kiriya, H.; Bulanov, S. V.; Bolton, P.; Sagisaka, A.; Oishi, Y.; Fujii, T.; Nemoto, K.; Kanazawa, S.; Kondo, S.; Okada, H.; Shimomura, T.; Noda, A.

The Laser Society of Japan

25 May 2011

TOKITA, Shigeki

Kondo Prize

“Studies on the Realization of Laser-accelerated Electron Bunch Compression and Its Application to Electron Diffraction”

Osaka University



10 May 2011

MIYASAKA, Yasuhiro

Presentation Award

The 31st Annual Meeting of the Laser Society of Japan

“Femtosecond Laser Nano-ablation Mechanism for Metals, Measurement of the Angular Distribution of Ion Emission”

The Laser Society of Japan



25 May 2011

Poster Awards

HIRANO, Toshiko



The Best Poster Presentation Award

The 28th Joint Symposium (The 78th Meeting of the Association of Organic Micro-Analysts in the Japan Society for Analytical Chemistry/The 86th Meeting of the Technical Committee on Measurement of Mechanical Quantities in the Society of Instrument and Control Engineers)

“Solution of Some Problems in the Determination of Sulfur and Halogens in Organic Compounds with the Fully-automatic System Using a Coupled Combustion/ion Chromatography (XS-100) –Investigation on Practical Conditions Not Described in the Manual–”

Organizing Committee of the 28th Joint Symposium

13 May 2011

MIEDA, Eiko



The Best Poster Award

The 15th Symposium of the Society of Silicon Chemistry, Japan

“Generation of Silylene Bearing Bulky Benzyl Substituent”

The Society of Silicon Chemistry, Japan

21 October 2011

SHIGETA, Takashi



Best Poster Award

41st Congress of Heterocyclic Chemistry

“Asymmetric Desymmetrization of σ -Symmetric Linear Diols by Organocatalytic Remote Chiral Recognition”

Organizing Committee of 41st Congress of Heterocyclic Chemistry

21 October 2011

HAMADA, Shohei



Best Poster Award

44th Symposium on Chemical and Biochemical Oxidation

“Development of a Novel Nitroxyl Radical Oxidation Catalyst”

Organizing Committee of 44th Symposium on Chemical and Biochemical Oxidation

5 November 2011

TAKEUCHI, Hironori



Best Poster Award

The 31st Seminar on the Society of Synthetic Organic Chemistry, Japan, Kinki Branch

“Concise Total Synthesis of Ellagitannins via Organocatalytic Regioselective Acylation”

The Society of Synthetic Organic Chemistry, Japan, Kinki Branch
16 November 2011

Outstanding C&FC 2011 Poster Presentation

International Symposium on Catalysis and Fine Chemicals 2011

“An Organocatalytic Regioselective Approach toward Short Total Syntheses of Tellimagrandin I and II”

Organizing Committee of Catalysis and Fine Chemicals 2011
7 December 2011

HYAKUTAKE, Ryuichi



Best Poster Award

The 31st Seminar on the Society of Synthetic Organic Chemistry, Japan, Kinki Branch

“Asymmetric Synthesis of β -Lactams by Intramolecular Conjugate Addition of Serine Derivatives via Memory of Chirality”

The Society of Synthetic Organic Chemistry, Japan, Kinki Branch
16 November 2011

AZUMA, Yusuke



The Best Poster Prize

SRM 2011 (21st Symposium on Role of Metals in Biological Reactions, Biology and Medicine)

“Selective Sensing of Nickel(II) by a Helical Peptide Bearing a Pair of Dipicolylamine Moieties”

The Pharmaceutical Society of Japan

30 May 2011

HIROSE, Hisaaki



The Best Poster Prize

The 48th Japanese Peptide Symposium

“Topical Migration of Membrane-associated Molecules Induced by Direct Influx of Arginine-rich Peptides into Cells”

The Japanese Peptide Society

29 September 2011

NOSHIRO, Daisuke



The Best Poster Prize

The 48th Japanese Peptide Symposium

“Metal-Mediated Leakage Control by Histidine-Containing Alamethicin Analogs”

The Japanese Peptide Society

29 September 2011

OSAKI, Katsuhiko



The Best Poster Prize

The 48th Japanese Peptide Symposium

“Creation of Artificial Epidermal Growth Factor Receptor Activated by Coiled-Coil Peptides”

The Japanese Peptide Society

29 September 2011

KIMURA, Hiroshi



Poster Presentation Award

34th Symposium on Solution Chemistry of Japan

“In situ Kinetic Study on Hydrothermal Reaction of D-Glucose Using NMR”

The Japan Association of Solution Chemistry

16 November 2011

MATSUO, Yushi



Poster Presentation Award

34th Symposium on Solution Chemistry of Japan
“Solution-State $^1\text{H-NMR}$ Study on Naphthalene Derivatives
in Lipid Membrane”

The Japan Association of Solution Chemistry

16 November 2011

KURITA, Yushi



The Best Presentation Award

The 2011 Autumn Meeting of the Society of Rheology, Japan
“Dielectric Investigation of Segmental Dynamics of
1,2-polybutadiene”

The Society of Rheology, Japan

6 October 2011

NAKAMURA, Makoto



The Poster Presentation Award

The 42nd Summer School of the Society of Fiber Science and
Technology, Japan

“Distribution of Glass Transition Temperature in Poly(methyl
methacrylate) Thin Films”

The Society of Fiber Science and Technology, Japan

30 August 2011

YAMADA, Yasuhiro



Poster Award (Gold Award)

7th International Symposium on Transparent Oxide Thin Films
for Electronics and Optics(TOEO-7)

“Band-Edge Luminescence From SrTiO_3 : No Polaron Effect”

Organizing Committee of TOEO-7

25 March 2011

HAMADA, Takanori



The Poster Presentation Award

The 42nd Summer School of the Society of Fiber Science and
Technology, Japan

“Structural Analysis of Isotactic Poly(methyl Methacrylate)
during the Induction Period of Crystallization by X-ray Scattering”

The Society of Fiber Science and Technology, Japan

30 August 2011

du VERLE, David



Best Poster Award 1st Prize

11th International Workshop on Bioinformatics and Systems
Biology (IBSB)

“Reverse-engineering Gene Regulatory Networks Using Time
Series”

Research Training Group “Computational Systems Biology”, DFG
(Deutsch Forschungsgemeinschaft, German Research Foundation)

20 July 2011

KAWASAKI, Yohji



The Best Presentation Award

The 2011 Annual Meeting of the Society of Rheology, Japan
“Component Dynamics of PI Chains in Grassy PI/PtBS Miscible
Blend”

The Society of Rheology, Japan

19 May 2011

Obituary

Professor Emeritus

Dr KITAMARU, Ryozo (1924–2011)



Dr. Ryozo Kitamaru, Professor Emeritus of Kyoto University, passed away unexpectedly on January 10, 2011, in Kyoto.

Dr. Ryozo Kitamaru was born in Kyoto on July 8, 1924. He graduated from Department of Fiber Chemistry, Faculty of Engineering, Kyoto University in 1947 and was employed in Mitsubishi Chemical Co., Ltd. After working in the company for one and a half year, he returned to Department of Fiber Chemistry, Kyoto University to continue his studies on fiber and polymer chemistry under the supervision of Professor Waichiro Tuji, Institute for Chemical Research, Kyoto University. In 1956, he was appointed Instructor in Institute for Chemical Research, Kyoto University and received a doctoral degree from Kyoto University for his studies on chemical treatment of cotton fiber in 1959. He was promoted to Associate Professor in the same Institute in 1960, and stayed in the laboratory of Professor Leo Mandelkern, Florida State University, USA, from October, 1962 to May, 1964 as a research associate to work on polymer crystallization. In 1987, Dr. Kitamaru was promoted to Full Professor of Kyoto University to hold the chair of fiber chemistry, or Laboratory of Fiber Chemistry, Institute for Chemical Research. Due to the reorganization of Institute for Chemical Research, he was appointed to the Chief Professor of the Laboratory of Fundamental Materials Science 1987. He retired from Kyoto University on March 31, 1989 and was honored with the title of Professor Emeritus of Kyoto University on April 1st, 1989.

Dr. Kitamaru performed extensive researches in both fundamental and applied fields of polymer science such as improvement of properties of natural and synthetic fiber, production of synthetic fiber, structure and dynamics of polymer materials using new experimental techniques such as solid-state nuclear magnetic resonance (NMR) and neutron scattering (NS). In particular, he obtained

prominent results in studying the structure of solid polymers using solid-state NMR, which were highly evaluated worldwide. Due to the high quality achievements in his researches, he was often invited to international conferences to give lectures. He published a textbook “NUCLEAR MAGNETIC RESONANCE: Principles and Theory” in both Japanese and English, which was also highly appreciated in this field.

In addition to researches, his achievements in education were outstanding. He gave lectures on polymer materials science at the Graduate School of Engineering, Kyoto University and he supervised dissertation works of not only many graduate students but also many foreign researchers from England, China and other countries. Moreover, he gave lectures in many universities such as Nagoya University, Fukui University, Kyoto Institute of Technology, Okayama University and Kyushu University as a visiting lecturer. For many years he presided the Poval Committee, which was established by Professor Emeritus Ichiro Sakurada, Kyoto University, soon after the Second World War II to investigate the applications of poly(vinyl alcohol). He organized the Research Group of Nuclear Magnetic Resonance in the Society of Polymer Science, Japan, the Advanced Fiber Material Committee, Fiber Society, Japan and the Society of Solid-State NMR for Materials, and served as a chair of their organizations.

Dr. Kitamaru was appointed Professor of Ryukoku University just after the retirement from Kyoto University until 1993 to give lectures at the Faculty of Science and Technology and to conduct researches on polymer science.

The Japanese Government made public recognition of his achievements by a medal, “Kun-Santo-Zuihosho” (the Third Order of the Sacred Treasure) in 2002 and a court rank, “Ju-shi-i” (the Junior Fourth Rank) in 2011.

Obituary

Professor Emeritus

Dr MIYAMOTO, Takeaki (1937–2011)



Dr. Takeaki Miyamoto, Professor Emeritus of Kyoto University, passed away on June 2, 2011, in Kyoto.

Dr. Miyamoto was born in Manchuria, China on April 3, 1937. He graduated from the Department of Fiber Chemistry at the Faculty of Engineering, Kyoto University in 1962 and continued his studies on polymer chemistry as a graduate student for two years. After 4 years of service at Nittobo Co. Ltd., he was appointed Instructor of the Laboratory of Polymer Properties headed by the late Professor Emeritus Hiroshi Inagaki at the Institute for Chemical Research, Kyoto University in 1968 and received a doctoral degree in 1970 from the Faculty of Engineering, Kyoto University for his studies on “Unperturbed Dimensions, Conformations & Steric Isomerisms of Polymer Chains”. On leave from the University, he made a stay in Freiburg University, (West) Germany in the years 1970 and 1971 to work on functional polymers in collaboration with Professor H.-J. Cantow. He was promoted to Associate Professor in 1977 at the Institute and to full Professor in 1988 to take charge of the Laboratory of Polymer Separation and Characterization (later renamed the Laboratory of Polymeric Materials). From April 1, 1994, he was appointed Director of the Institute for two years and made quite a few important contributions not only to the Institute but also to the University. He retired from Kyoto University in 2000, one year earlier than expected, and was honored with the title of Professor Emeritus of Kyoto University. Subsequently, he served 6 years as Principal in Matsue National College of Technology, and for his great achievements on the management and administration, he was honored with the title of Professor Emeritus of Matsue National College of Technology in 2006.

Dr. Miyamoto’s research interest encompassed a wide array of the science and technology of functional polymers and fiber materials. His scientific life started with the synthesis and solution-property study of block copolymers. With a number of achievements in these fundamental fields of polymer science, his interest was directed to

polymer materials in general, above all, to naturally occurring polymers. He established a method to characterize the second-order structure of wool keratin by circular dichroic spectroscopy, with which he succeeded in disclosing details of the $\alpha\beta$ transition of the component protein. He was the first to perform a detailed study on the interactions between wool keratin and metal ions by means of gel chromatography. This fundamental work led him to develop waste wool-based new materials like a heavy-metal adsorbent and a cosmetic substrate. He is also known as a distinguished cellulose scientist, in particular for his studies on the characterization of the substituent distributions along the chain in cellulose derivatives and the effects of these distributions on their physical and physicochemical properties. He also developed systematic work to elucidate the relationships between the molecular structure and functions such as liquid crystallinity in cellulose derivatives. For his brilliant achievements, he was awarded in 1983 the Prize of Fiber Science and Technology, Japan.

He also devoted himself to the Society of Fiber Science and Technology, Japan as President for the years 1995 and 1996, and to the Cellulose Society of Japan as President for the years 1997 and 1998. He was awarded by each of these Societies for his distinguished services to them. He was chair or a member of organizing committee in a number of international scientific conferences/symposiums and made no less contributions to the promotion of international collaboration in polymer science, in particular with Germany and China. He was honored in 2004 with the title of Professor Emeritus of Donghu College, Wuhan University, China.

His sincere and warm personality was respected by many friends, colleagues, students, and all those who came in contact with him. He educated and mentored a lot of capable students and scientists. The Government made public recognition of his achievements by the Order of the Sacred Treasure, “Zuihouchujushou” medal and granted the Senior Grade of the Fourth Court Rank in 2011.

Obituary

Professor Emeritus

Dr FUJITA, Eiichi (1922–2011)



Dr. Eiichi Fujita, Professor Emeritus of Kyoto University, passed away on July 24, 2011, in Kyoto.

Dr. Eiichi Fujita was born in Osaka on February 2, 1922. He graduated from Department of Pharmaceutical Sciences, Faculty of Medicine, Kyoto Imperial University in 1943. After the graduation, he was appointed a researcher in the Faculty of Medicine, Kyoto Imperial University in 1943. In the same year, he moved to navy as a pharmacy officer and was there until 1945. He joined the Faculty of Medicine, Kyoto Imperial University as a researcher in 1946. He was appointed Associate Professor of the Faculty of Pharmaceutical Sciences, Tokushima University, in 1951. He received a doctoral degree from Kyoto University for the study on biologically active alkaloids, terpenoids, and peptides. In 1954, he was promoted to be Professor of Tokushima University. In 1962, Dr. Fujita was appointed Professor of Institute of Chemical Research, Kyoto University to direct the Laboratory of Physiologically Active Compounds. From April 1, 1982 to March 31, 1984, he was appointed Director of the Institute and made great contributions to the development of the Institute and Kyoto University. He retired from Kyoto University and received the title of Professor Emeritus of Kyoto University in 1985. After the retirement, Dr. Fujita served as President of Osaka University of Pharmaceutical Sciences from 1985 to 1991, and he made great contributions to the development of Osaka University of Pharmaceutical Sciences including the relocation of the University to the current Takatsuki Campus. He also served as Councillor of Institute for Molecular Science, National Institutes of Natural Sciences, from 1987 to 1993.

Dr. Fujita conducted extensive researches in both natural product chemistry and synthetic organic chemistry. He

has achieved creative works on biologically active natural products, asymmetric synthesis, and antitumor agents. In particular, he has achieved isolation and total syntheses of biologically active alkaloids, terpenoids, and peptides. He has developed a series of asymmetric reactions including asymmetric desymmetrization of σ -symmetric dicarboxylic acids by chiral sulfur reagents, new synthetic methods employing silicon- and tin chemistry, selective bond cleavage reactions based on a hard acid-soft nucleophile system, and efficient radiosensitizers for tumor treatment. He also achieved total synthesis of various biologically active natural products. Since these achievements were highly appreciated internationally as well as domestically, he was frequently invited to International Conference on Natural Products, IUPAC Symposium, International Conference on Heterocyclic Chemistry, European Conference on Stereochemistry, and so on. For his brilliant achievements on natural product chemistry, he was awarded the Pharmaceutical Society of Japan Award in 1978.

Dr. Fujita was an active member of the Pharmaceutical Society of Japan, the Society of Synthetic Organic Chemistry of Japan, the Chemical Society of Japan, and so on. He served as President of the Kinki branch of the Pharmaceutical Society of Japan in 1980 and as President of the Society of Synthetic Organic Chemistry, Kansai branch, Japan in 1984.

Dr. Fujita was a gentle, sincere, and warmhearted man. He educated and mentored a lot of capable students and scientists. A large number of Professors have been produced from his laboratory. The Japanese Government made the public recognition of his achievement by the Second Class of the Order of the Sacred Treasure, “Kun-Ni-tou Kyokujitsu Zuihoushou” Medal in 1996.



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

SELECTED GRANTS

THESES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Mieda, E.; Sasamori, T.; Sase, S.; Goto, K.; Tokitoh, N., Formation of a Unique Fluorosilene—KF Complex Bearing Bulky Substituents, *Chem. Lett.*, **40**, 196-197 (2011).

Sasamori, T.; Mieda, E.; Tokitoh, N., Unexpected Formation of Dihydrobenzosilole Derivative via the Intramolecular Cyclization in the Reaction of Overcrowded Dichloromethylsilane with Aryllithium, *Heterocycles*, **82**, 1103-1112 (2011).

Mizuhata, Y.; Tokitoh, N., Chemistry of Aromatic Compounds Containing a Heavier Group 14 Element, *J. Synth. Org. Chem. Jpn.*, **69**, 691-704 (2011) (in Japanese).

Sasamori, T.; Sugamata, K.; Tokitoh, N., Halogenation Reactions of a Ditelluride Having Bulky Aryl Groups Leading to the Formation of Organotellurium Halides, *Heteroatom Chem.*, **22**, 405-411 (2011).

Sugamata, K.; Sasamori, T.; Tokitoh, N., Fluorination Reaction of a Ditelluride Bearing Bulky Aryl Substituents: Formation of Mixed-Valent Te(IV)—Te(II) Ditelluride Difluoride, *Chem. Asian J.*, **6**, 2301-2303 (2011).

Tokitoh, N.; Yuasa, A.; Sasamori, T., Chalcogenation of 1,2-Bis(ferrocenyl)disilene: The First Isolation of 1,2,3,4-Dithiadisiletane, *Phosphorus, Sulfur, and Silicon and the Related Elements*, **186**, 1217-1219 (2011).

Tokitoh, N.; Inamura, K.; Mizuhata, Y., New Aspects in the Coordination Chemistry of Ge- and Sn-Containing Metallaaromatic Compounds, *Phosphorus, Sulfur, and Silicon and the Related Elements*, **186**, 1323-1325 (2011).

Tsurusaki, A.; Sasamori, T.; Wakamiya, A.; Yamaguchi, S.; Nagura, K.; Irlle, S.; Tokitoh, N., Synthesis of 1-Phospha-2-boraacenaphthenes: Reductive 1,2-Aryl Migration of 1-Diarylboryl-8-dichlorophosphinonaphthalenes, *Angew. Chem. Int. Ed.*, **50**, 10940-10943 (2011).

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Han, J. S.; Sasamori, T.; Mizuhata, Y.; Tokitoh, N., Evidence for a LiBr-Assisted Generation of a Silylene from a 1,2-Diaryl-1,2-dibromodisilene, *Chem. Asian J.*, **6**, 2301-2303 (2011).

Agou, T.; Sebastian, M.; Lescop, C.; Reau, R., Folding of a Coordination Polymer Framework Incorporating Swiveling Pins Driven by π - π Interactions, *Inorg. Chem.*, **50**, 3183-3185 (2011).

Perez, A. I. A.; Biet, T.; Graule, S.; Agou, T.; Lescop, C.; Branda, N. R.; Crassous, J.; Reau, R., Assembling N₂P₂N Pincers for Coordination-Driven Synthesis of Supramolecular [2,2]Paracyclophane Analogues, *Chem. Eur. J.*, **17**, 1337-1351 (2011).

Kimura, T.; Iwama, T.; Namao, T.; Suzuki, E.; Fukuda, T.; Kobayashi, N.; Sasamori, T.; Tokitoh, N., Preparation and Characterization of Nonclassical Tetraazaporphyrin, Bis(4-methylpyridine)[1,3,5,7,9,11,13,15-octaphenyltetra(3,4-thieno)-tetraazaporphyrinato]ruthenium(II), *Eur. J. Inorg. Chem.*, 888-894 (2011).

Segawa, Y.; Miyamoto, S.; Omachi, H.; Matsuura, S.; Senel, P.; Sasamori, T.; Tokitoh, N.; Itami, K., Concise Synthesis and Crystal Structure of [12]Cycloparaphenylene, *Angew. Chem. Int. Ed.*, **50**, 3244-3248 (2011).

— Structural Organic Chemistry —

Han, A.; Bai, J.; Murata, Y.; Komatsu, K., Synthesis and Characterization of the Fullerene-Terthiophene Dyads, *Heteroatom Chem.*, **22**, 72-78 (2011).

Shang, M.; Warren, R. N.; Butler, D. N.; Murata, Y.; Margetic, D., Synthesis of Bis-peptides Attached on Poly[n]norbornane Molecular Scaffolds with Well-defined Relative Positions and Distances, *Mol. Divers.*, **15**, 541-560 (2011).

Nambo, M.; Segawa, Y.; Wakamiya, A.; Itami, K., Selective Introduction of Organic Groups to C₆₀ and C₇₀ Using Organoboron Compounds and Rhodium Catalyst: A New Synthetic Approach to Organo(hydro)fullerenes, *Chem. Asian J.*, **6**, 590-598 (2011).

Li, Y.; Lei, X. -G.; Lawler, R.; Murata, Y.; Komatsu, K.; Turro, N., Distance-dependent Para-H₂→Ortho-H₂ Conversion in H₂@C₆₀ Derivatives Covalently Linked to a Nitroxide Radical, *J. Phys. Chem. Lett.*, **2**, 741-744 (2011).

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Yamada, Y.; Kanemitsu, Y., Photocarrier Recombination Dynamics of SrTiO₃, *Proceedings of SPIE*, **7937**, [793710-1]-[793710-8] (2011).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

Australian Nuclear Science and Technology Organization, Bragg Institute

Central Queensland University, Centre for Molecular Architecture

The University of Sydney, Key Centre for Polymers & Colloids, School of Chemistry

[Austria]

University of Natural Resources and Life Sciences, Department of Chemistry

[Canada]

University of Calgary, Department of Chemistry

[China, P.R.]

Fudan University, School of Computer Science

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Normal University, Shenyang, College of Chemistry and Life Science

Peking University, College of Life Sciences

Tsinghua University

University of Science and Technology of China, Department of Chemistry

[Croatia]

Ruder Bošković Institute, Division of Organic Chemistry and Biochemistry

[Czech]

Academy of Sciences of the Czech Republic, Institute of Organic Chemistry and Biochemistry

[Estonia]

National Institute of Chemical Physics and Biophysics

[Finland]

Tampere University of Technology, Department of Chemistry and Bioengineering

[France]

Institut Laue-Langevin

[Germany]

European Molecular Biology Laboratory, Structural and Computational Biology Research Unit

Friedrich-Alexander-Universität, Interdisciplinary Center for Molecular Materials

Max-Planck-Institut für Kernphysik

Philipps University, Material Sciences Center

[India]

The M. S. University of Baroda, Applied Chemistry Department, Faculty of Technology and Engineering

[Indonesia]

University of Bengkulu, Department of Chemistry

[Korea, R.]

Gwangju Institute of Science and Technology, Department of Nanobio Materials and Electronics and School of Materials Science and Engineering

[Netherlands]

TU Delft, Reactor Institut Delft

[Russia]

Joint Institute for Nuclear Research

[Sweden]

Karolinska Institutet, Division of Physiological Chemistry II

Lund University, Department of Chemical Physics

Stockholm University, Department of Biochemistry and Biophysics

[Taiwan]

National Tsing-Hua University, Department of Physics and Institute of Nanoengineering and Microsystems

[Thailand]

Suranaree University of Technology, Institute of Science

[U.K.]

Newcastle University, School of Chemistry

University of Cambridge, Cavendish Laboratory

University of Southampton, School of Chemistry

[U.S.A.]

Argonne National Laboratory

Boston University School of Medicine, The Pulmonary Center

Brown University, Department of Chemistry

Columbia University, Department of Chemistry

Lawrence Berkeley National Laboratory

Louisiana Tech University, Institute for Micromanufacturing

State University of New York at Stony Brook, Department of Chemistry

Temple University, Department of Chemistry

University of California, Ocean Sciences Department

University of Hawaii, Department of Oceanography

University of Miami, Department of Chemistry

University of Pennsylvania, Department of Materials Science and Engineering and Laboratory for Research on the Structure of Matter

Yale University, Department of Molecular, Cellular and Developmental Biology

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Tokitoh, N.

Construction of Polycyclic Aromatic Compounds Containing Heavier Group 14 Elements and Development of Their Functions by Utilizing the Features of Main Group Elements
Grants-in-Aid for Scientific Research (B)
1 April 2010–31 March 2013

Sasamori, T.

Construction of Novel d- π Conjugated Systems Containing Heavier Main Group Elements and Their Functions
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

Mizuhata, Y.

Construction of Novel Silicon–Silicon Double-Bond Compounds Bearing Alkynyl Substituents
Grants-in-Aid for Young Scientists (B)
1 April 2009–31 March 2012

Mizuhata, Y.

Syntheses of Polycyclic Aromatic Compounds Containing Heavier Group 14 Elements and Their Functions
Kinki Invention Center
1 April 2010–31 March 2011

Mizuhata, Y.

Synthesis of Phthalocyanine Derivatives Bearing Phosphorus Atoms as Skeletal Elements and Their Properties
Grants-in-Aid for Scientific Research on Innovative Area “ π -Space”
1 April 2011–31 March 2013

Agou, T.

Development of Electron-accepting Conjugated Molecules Densely Substituted with Boron Atoms
Grants-in-Aid for Young Scientists (B)
1 April 2009–31 March 2011

Kawashima, T.; Kobayashi, J.; Agou, T.

Development of Dimensionally-Extended Hetero- π -conjugated Molecules
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

— Structural Organic Chemistry —

Murata, Y.

Synthesis and Properties of Bowl-shaped π -Systems by Top-down Approach
Grants-in-Aid for Young Scientists (A)
1 April 2008–31 March 2011

Murata, Y.

Creation and Function of Spherical π -Space Encapsulating an Active Small Molecule
Grants-in-Aid for Scientific Research on Innovative Areas “ π -Space”
1 December 2008–31 March 2013

Murata, Y.

Synthesis of Tailor-made Nanocarbons and Their Application to Electronic Devices
Grants-in-Aid for Scientific Research (A)
1 April 2011–31 March 2016

Wakamiya, A.

Creation of π -Electron Boron Clusters Using Lewis Basic Ligand
Grants-in-Aid for Challenging Exploratory Research
1 April 2009–31 March 2011

Wakamiya, A.; Murata, Y.

Development of Dye-sensitized Solar Cells Using Organic Dyes Derived from Natural Products
ALCA (Advanced Low Carbon Technology Research and Development Program), Japan Science and Technology Agency
1 October 2011–31 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), Japan Science and Technology Agency
1 October 2010–31 March 2016

Murata, M.

Construction of Spherical Conjugated π -Electron Systems and Elucidation of Their Functions
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2012

— Synthetic Organic Chemistry —

Kawabata, T.

Fine Organic Synthesis Based on Catalytic Regioselective Functionalization
Grants-in-Aid for Scientific Research (A)
1 April 2009–31 March 2013

Kawabata, T.

Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grants-in-Aid for Scientific Research on Innovative Area
1 October 2011–31 March 2015

Furuta, T.

Development of Regio- and Stereoselective Transformations of Polyfunctionalized Molecules with Axially Chiral Catalysts
Grants-in-Aid for Scientific Research (C)
28 April 2011–31 March 2014

Yoshimura, T.

Syntheses of Novel Amino Acids and Natural Products Derived from Amino Acids via Memory of Chirality
Grants-in-Aid for Young Scientists (B)
28 April 2011–31 March 2013

—Advanced Inorganic Synthesis—

Teranishi, T.
Development of Photoacoustic Gold Nanoparticle Probes for Cancer Detection
Industry-Academia Collaborative R&D Program
1 December 2011–31 March 2017

Teranishi, T.
Creation of Enhanced Photoelectric Fields Based on Nanoparticle Superlattices for Novel Chemical Reactions
Grants-in-Aid for Scientific Research on Priority Area “Strong Photon-Molecule Coupling Fields”
1 August 2007–31 March 2011

Teranishi, T.
Development of Structure-Specific Energy-Related Functional Materials Using Heterostructured Nanoparticles
Grants-in-Aid for Scientific Research (A)
1 April 2011–31 March 2014

Teranishi, T.
Elucidation of Crystal Structure-Dependent Hydrogen Storage Properties of Large Palladium Nanoparticles
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2012

Teranishi, T.
Synthesis of Macrocyclic π -Conjugated Ligand-Protected Gold Clusters and Fabrication of Nano-Gap Single Electron Devices
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2008–31 March 2014

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Tsujii, Y.
Fabrication and Precise Characterization of Novel Tribomaterials
Grants-in-Aid for Scientific Research (A)
1 April 2009–31 March 2012

Tsujii, Y.
Development of Novel Nanosystem by Hierarchically Assembling Concentrated Polymer Brushes
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2009–31 March 2015

Tsujii, Y.
Research and Development of Safe Solid-Electrolyte by Hybridization of Ionic Liquids and Polymers
Research and Development for Promotion of Regional Innovation Program, Japan Science and Technology Agency
9 August 2010–31 March 2012

Ohno, K.
Development of Next-Generation MRI Contrast Agent
Industrial Technology Research Grant Program, NEDO
1 July 2009–30 June 2013

— Polymer Controlled Synthesis —

Yamago, S.
Creation of Hoop-shaped π -conjugated Molecules through the Supramolecular Chemical Approach and Elucidation of Their Properties
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2010–31 March 2016

— Inorganic Photonics Materials —

Yoko, T.
Organic-inorganic Material for Biosensor Application
Grants-in-Aid for Science Research, Challenging Exploratory Research
1 April 2011–31 March 2014

Tokuda, Y.
Self-organization Synthesis of Nano-tube for Biosensor Application
Sumitomo Foundation, Grant for Basic Science Research Projects
1 November 2011–31 March 2013

Masai, H.
Study on Emission Mechanism of Sn-doped Low-melting Glass and the Application
Asahi Glass Foundation, Research Grant Program
1 April 2011–31 March 2012

Masai, H.
Application of Tin-doped Low-melting Glass to Novel Emission Material
Inamori Foundation, Research Grant
1 April 2011–31 March 2013

— Nanospintronics —

Ono, T.
Development of Novel Spin Dynamics Devices
Grants-in-Aid for Scientific Research(S)
1 April 2011–31 March 2016

Kobayashi, K.
Nonequilibrium Many-body Dynamics in Solid State Devices
Funding program for Next Generation World-Leading Researchers (NEXT program)
10 February 2011–31 March 2014

Chiba, D.
Realization of Electric-field-induced Magnetization Switching and its Application for Information Writing Method in Nano-scaled Magnetic Non-volatile Memories
PRESTO Program “Nanosystem and Function Emergence”, Japan Science and Technology Agency
1 October 2010–31 March 2014

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
Novel Methods for Delivering Nucleic Acids Therapeutics
Japan Science and Technology Agency, Strategic Japanese-Swedish Cooperative Programme on “Multidisciplinary BIO”
1 July 2009–30 June 2012

— **Chemistry of Molecular Biocatalysts** —

Hiratake, J.
Applications of Cellular Collagen Biosynthesis Induced by Novel γ -Glutamyl Transpeptidase (GGT) Inhibitors
Adaptable and Seamless Technology Transfer Program through Target-Driven R&D (A-STEP), Japan Society and Technology Agency
1 December 2009–31 March 2012

Watanabe, B.
Development of Novel Chemicals to Regulate Glutathione Biosynthesis
Grants-in-Aid for Young Scientists (Start-up)
1 April 2009–31 March 2011

Koeduka, T.
Isolation and Characterization of Prenyltransferases in Furano-coumarin Biosynthesis
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2011

— **Molecular Biology** —

Aoyama, T.
Mechanism of Cytokinin Signal Transduction by the Response Regulator ARR1
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

Aoyama, T.
Growth Strategy of Plants through Morphological Changes of Roots
Grants-in-Aid for Scientific Research on Innovative Area
1 April 2011–31 March 2013

Tsuge, T.
Regulatory Mechanism of Plant Morphogenesis by the Regulator of mRNA Metabolism SAP130
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

Tsuge, T.
Regulatory Mechanism of Environmental Stimuli Response that Integrates mRNA Metabolism and Protein Degradation in the Cell
Grants-in-Aid for Scientific Research on Innovative Area
1 April 2011–31 March 2013

— **Chemical Biology** —

Uesugi, M.
Control and Analysis of Cells by Synthetic Small Molecules
Funding Program of Next Generation World-Leading Researchers (NEXT Program)
10 February 2011–31 March 2014

DIVISION OF ENVIRONMENTAL CHEMISTRY

— **Molecular Materials Chemistry** —

Kaji, H.
Fabrication of High-Performance Polymer EL Devices Having Covalently-Bonded Interfaces
Grants-in-Aid for Scientific Research (A)
1 April 2009–31 March 2012

Kaji, H.
Development of Solid-State NMR Methodology for the Structure Analysis of Donor-Acceptor Supramolecules
Grants-in-Aid for Challenging Exploratory Research
1 April 2009–31 March 2010

Goto, A.
Development of Green Living Radical Polymerization with Low Cost and Elucidation of Their Properties
Industrial Technology Research Grant Program, NEDO
10 September 2007–31 August 2011

Goto, A.
Dual Control Living Polymerizations with Organic Catalysts
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

Goto, A.
High Performance Color Material by Living Radical Polymerization with Organic Catalysts
Japan Science and Technology Agency, A-STEP
1 November 2011–31 March 2015

— **Hydrospheric Environment Analytical Chemistry** —

Sohrin, Y.
Development of Precise Isotopic Analysis for Founding Heavy Stable Isotopic-Marine Chemistry
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

Sohrin, Y.
Development of Marine Geochemistry of Palladium, Platinum and Gold
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2012

Sohrin, Y.
Development of a New Automated System for Preconcentration of Heavy Metals to Assess the Influence of Biology and Its Application to Oceanographic Study
Steel Foundation for Environmental Protection Technology
1 November 2011–31 October 2013

Murayama, M. (Investigator: Sohrin, Y.)
Reconstruction of Redox Conditions in Meedee Lake, Mediterranean, Sediment Core Using Molybdenum/Tungsten Ratio
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

— **Solution and Interface Chemistry** —

Hasegawa, T.
Operando Analysis of Concentration and Diffusion of Negatively-Adsorptive Chemical Species in a Monolayer Formed at an Air/Water Interface
Grants-in-Aid for Scientific Research on Innovative Areas “Molecular Sciences of Soft Interface”
1 April 2011–31 March 2013

Matubayasi, N.
Free-Energy Analysis of ATP Hydrolysis
Grants-in-Aid for Scientific Research on Innovative Areas “Hydration and ATP Energy”
1 December 2008–31 March 2013

—Molecular Microbial Science—

Kurihara, T.
Exploration of Cold-Adapted Microorganisms for Development of New Low-Temperature Biotechnological Processes
Grants-in-Aid for Scientific Research (B)
1 April 2010–31 March 2013

Kurihara, T.
Investigation of Chaperone Function of Phospholipids Containing Polyunsaturated Fatty Acids and Their Application to Overproduction of Membrane Proteins
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2012

Kurihara, T.
Biosynthesis and Function of Phospholipids Containing Polyunsaturated Fatty Acids in Bacteria
Grant from Japan Foundation for Applied Enzymology
1 April 2011–31 March 2012

Kawamoto, J.
Development of a System for the Bioremediation of Rare Metal Pollution and Rare Metal Recovery Using Novel Metal-Metabolizing Bacteria
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

Kawamoto, J.
Synthesis of Functional Metal Nanoparticles by Using Metal-Metabolizing Bacteria
Grants-in-Aid for Challenging Exploratory Research
1 April 2011–31 March 2013

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

—Polymer Materials Science—

Kanaya, T.
Polymer Crystallization and Control of Higher Order Structure Control through Non-equilibrium Intermediate States
Grants-in-Aid for Scientific Research (A)
1 April 2008–31 March 2012

Nishida, K.
Property Control of Water-soluble Cellulose Derivatives
Grants-in-Aid for Scientific Research (C)
1 April 2011–31 March 2014

Inoue, R.
Surface and Interfacial Physical Properties of Polymer Thin Films Studied by Neutron Scattering
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2012

—Molecular Rheology—

Watanabe, H.
Creation of Non-equilibrium Soft Matter Physics: Structure and Dynamics of Mesoscopic Systems
Grants-in-Aid for Scientific Research on Priority Areas “Creation of Non-Equilibrium Soft Matter Physics”
1 April 2006–31 March 2011

Watanabe, H.
Effect of Thermodynamical and Geometrical Constraints on the Dynamics of Block-copolymers
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

Masubuchi, Y.
Multi-scale Simulations for Soft Matters
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2006–31 March 2012

Masubuchi, Y.
A Novel Molecular Model for Branched Polymer Dynamics
Grants-in-Aid for Scientific Research (B)
1 April 2008–31 March 2011

Masubuchi, Y.
Relaxation of Polymers under Fast Flows
Grants-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

Matsumiya, Y.
Analysis of Mechanical Properties for Multi-component Liquid by Dielectric Methods
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2013

Uneyama, T.
Theory of Mechanical and Dielectric Response of Polymers under Shear Flow
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2013

—Molecular Aggregation Analysis—

Yoshida, H.
Inverse-Photoemission Spectroscopy with Zero Kinetic Energy Electrons for Measuring the Unoccupied Electronic States of Organic Semiconductors
PRESTO Program, Japan Science and Technology Agency
1 October 2009–30 September 2012

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

—Laser Matter Interaction Science—

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Electrons Accelerated in Plasmas by an Intense Femtosecond Laser
Grants-in-Aid for Scientific Research (S)
1 April 2011–31 March 2016

Sakabe, S.
High Energy Electron Gun of a Fine Wire Driven by an Intense Femtosecond Laser
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2012

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Plasma Electrons Produced by an Intense Femtosecond Laser
Yamada Science Foundation
1 April 2010–31 March 2012

Hashida, M.
Amorphous Metal Thin Film with the Surface of Periodic Nano-structures Self-formed by Femtosecond Laser Pulses
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

Tokita, S.
Development of Short-pulse Intense Laser Technology in Mid-infrared Fluoride Fiber Lasers
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2012

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

—Organic Main Group Chemistry—

Nakamura, M.
Development of Selective Organic Synthesis Based on Iron Catalysis
Funding Program for Next Generation World-Leading Researchers (NEXT Program)
1 March 2011–31 March 2014

Hatakeyama, T.
Synthesis of Helical π -Conjugated Molecules toward Next Generation Semiconductors
PRESTO Program, Japan Science and Technology Agency
1 October 2011–31 March 2014

—Advanced Solid State Chemistry—

Shimakawa, Y.
Strategic State-of-the-art Solid State Chemistry for New Functional Materials: Exploring for New Multi-functional Materials
Grants-in-Aid for Creative Scientific Research
1 April 2007–31 March 2012

Shimakawa, Y.
Exploring for New Functional Materials with Unusual Ionic States and Coordinations
Creation of Innovative Functions of Intelligent Materials on the Basis of the Element Strategy
1 April 2011–31 March 2016

—Organotransition Metal Chemistry—

Ozawa, F.
Study of C–H Direct Arylation Reactions for Precisely Controlled Synthesis of π -Conjugated Polymers
Grants-in-Aid for Science Research (B)
1 April 2011–31 March 2015

Nakajima, Y.
Efficient Photoreduction of Carbon Dioxide Catalyzed by an Iron Complex Bearing a Phosphaalkene Ligand
PRESTO Program, Japan Science and Technology Agency
1 October 2009–31 March 2013

—Photonic Elements Science—

Kanemitsu, Y.
Microscopic Spectroscopy of Highly Excited State in Semiconductor Nanostructures and Exploring Novel Optical Functionality
Grants-in-Aid for Scientific Research on Innovative Areas "Optical Science of Dynamically Correlated Electrons"
13 November 2008–31 March 2013

Tayagaki, T.
Controlling of the Many-body Interaction between Photoexcited Carriers toward Hot Carrier Solar Cells
PRESTO Program, Japan Science and Technology Agency
1 October 2009–31 March 2013

BIOINFORMATICS CENTER

—Chemical Life Science—

Kanehisa, M.
Deciphering Systemic Biological Functions by Integration of Genomic and Environmental Information
Bioinformatics Research and Development, Japan Science and Technology Agency
1 April 2006–31 March 2011

Kanehisa, M.
Genome-based Integrated Resource of Diseases, Drugs, and Environmental Substances
Life Science Database Integration Project, Japan Science and Technology Agency
1 April 2011–31 March 2014

Goto, S.
Hierarchical Structuring and Integration of Knowledge in Life Sciences
Integrated Database Project
1 April 2007–31 March 2011

Goto, S.
Key Technology Development for Data Integration and Application to Emerging Fields
Life Science Database Integration Project, Japan Science and Technology Agency
1 April 2011–31 March 2014

Goto, S.
System Biology Approach to Understanding Atherosclerosis
Japan – Sweden Research Cooperative Program, JSPS
1 April 2010–31 March 2012

—Mathematical Bioinformatics—

Akutsu, T.; Kawabata, T.; Nagamochi, H.; Hayashida, M.
An Approach to Novel Structural Design by Combining Discrete Methods and Kernel Methods
Grants-in-Aid for Scientific Research (A)
1 April 2010–31 March 2015

Akutsu, T.
Discrete Model-Based Methods for Control of Complex Biological Systems
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2013

THESES

AKI, Shiori
D Sc, Kyoto University
“Functional Analyses of *SAP130* Gene in *Arabidopsis thaliana*”
Supervisor: Prof AOYAMA, Takashi
26 September 2011

CHEN, Quan
D Eng, Kyoto University
“Component Dynamics in Miscible Polymer Blends and Block Copolymers”
Supervisor: Prof WATANABE, Hiroshi
25 March 2011

FUKATSU, Daisuke
D Pharm Sc, Kyoto University
“Synthesis and Properties of Functional Molecules with a BINOL Skeleton”
Supervisor: Prof KAWABATA, Takeo
23 March 2011

HAYASHI, Kazuhiro
D Pharm Sc, Kyoto University
“Creation of Axially Chiral Binaphyryl Surrogates with an Intramolecular Hydrogen Bond and its Application to Novel Organometallic Catalysis”
Supervisor: Prof KAWABATA, Takeo
23 March 2011

HIDese, Ryota
D Agr, Kyoto University
“Studies on Bacterial Dihydropyrimidine Dehydrogenases”
Supervisor: Assoc Prof KURIHARA, Tatsuo
23 March 2011

KAYAHARA, Eiichi
D Eng, Kyoto University
“Studies on the Precision Control of Polymer Structure Based on Heteroatom-Mediated Living Radical Polymerization Reaction”
Supervisor: Prof YAMAGO, Shigeru
23 March 2011

KHAMBUR, Bilon
D Med Sc, Kyoto University
“Translational Repression Stabilizes Messenger RNA of Autophagy-Related Genes”
Supervisor: Prof UESUGI, Motonari
24 December 2011

KONDO, Kouta
D Sc, Kyoto University
“Magnetic Domain Wall Dynamics in Ferromagnetic Nanowires”
Supervisor: Prof ONO, Teruo
24 March 2011

MATSUNAGA, Ryusuke
D Sc, Kyoto University
“Exciton Fine Structures in Semiconductor Carbon Nanotubes”
Supervisor: Prof KANEMITSU, Yoshihiko
23 March 2011

MIEDA, Eiko
D Sc, Kyoto University
“Studies on the Synthesis of Kinetically Stabilized Silyne”
Supervisor: Prof TOKITOH, Norihiro
23 March 2011

NAKAMURA, Atsushi
D Pharm Sc, Kyoto University
“Creation of Artificial Zinc Finger Transcription Factors Controlling the Cellular Circadian Clock”
Supervisor: Prof FUTAKI, Shiroh
23 March 2011

NAKAMURA, Shuji
D Sc, Kyoto University
“Nonequilibrium Quantum Transport in Semiconductor Mesoscopic Systems”
Supervisor: Associate Prof KOBAYASHI, Kensuke
24 March 2011

NAKAMURA, Yoshitaka
D Sc, Kyoto University
“Crystal Structure and Piezoelectric Properties of Bi-based Perovskite Thin Films”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2011

NOMURA, Akihiro
D Eng, Kyoto University
“Fundamental and Applied Studies on Friction/Lubrication of Concentrated Polymer Brushes”
Supervisor: Prof TSUJII, Yoshinobu
25 July 2011

POOLSAP, Unyanee
D Inf, Kyoto University
“Computational Methods for Predictions of RNA Pseudoknotted Secondary Structures and RNA-RNA Interactions”
Supervisor: Prof AKUTSU, Tatsuya
15 June 2011

SONOMURA, Kazuhiro
D Pharm Sc, Kyoto University
“Development of Novel Sequence Analysis Methods for the Elucidation of Protein Terminal Sequences Using Selective Modification of Alpha-Amino Groups”
Supervisor: Prof FUTAKI, Shiroh
25 July 2011

SUMIYA, Eiko
D Med Sc, Kyoto University
“Cell-Morphology Profiling of a Natural Product Library Identifies Bisebromoamide and Miuraenamide A as Actin Filament Stabilizers”
Supervisor: Prof UESUGI, Motonari
23 May 2011

TAKAYAMA, Kentaro
D Pharm Sc, Kyoto University
“Development of Efficient Intracellular Delivery Using Arginine-
Rich Peptides”
Supervisor: Prof FUTAKI, Shiroh
23 March 2011

YAMADA, Keisuke
D Sc, Kyoto University
“Dynamics of Current-Induced Magnetic Vortex Core”
Supervisor: Prof ONO, Teruo
24 March 2011

YAMADA, Tomonori
D Eng, Kyoto University
“Molecular and Electronics Structures and Charge-Transport
Properties of Triphenylamine-Related Materials for Organic Light-
Emitting Diodes (OLEDs)”
Supervisor: Prof KAJI, Hironori
25 July 2011

YOSHIDA, Keisuke
D Pharm Sc, Kyoto University
“Organocatalytic Regioselective Acylation via Recognition of
the Distance between Functional Groups”
Supervisor: Prof KAWABATA, Takeo
23 March 2011



THE 111TH
ICR ANNUAL
SYMPOSIUM

SEMINARS

MEETINGS AND
SYMPOSIA



THE 111TH ICR ANNUAL SYMPOSIUM

(9 December 2011)

ORAL PRESENTATIONS

MURATA, Michihisa (Structural Organic Chemistry)
“Synthesis, Aromaticity, and Optoelectronic Properties of Fullerene Derivatives”

MASUBUCHI, Yuichi (Molecular Rheology)
“Prediction of Rheology of Polymers”

MURDEY, Richard (Molecular Aggregation Analysis)
“Growth and in situ Electrical Measurements of Organic Semiconductor Thin Films”

KAWABATA, Takeo (Synthetic Organic Chemistry)
“Regioselective Functionalization of Polyols by Organocatalysis”

HIRATAKE, Jun (Chemistry of Molecular Biocatalysts)
“Something Unexpected: γ -Glutamyltranspeptidase Inhibitors and Collagen”

OGAWA, Tetsuya (Electron Microscopy and Crystal Chemistry)
“Cryo-TEM Observation of Organic Materials and Aggregates in Solution”



TAYAGAKI, Takeshi (Photonic Elements Science)
“Electron-Hole Dynamics and Optoelectronic Properties in Semiconductor Nanostructures”

– ICR Award for Young Scientists –
IMANISHI, Miki (Biofunctional Design-Chemistry)
“Control of Circadian Phase by an Artificial Zinc Finger Transcription Regulator”


– ICR Award for Graduate Students –
IWAMOTO, Takahiro (Polymer Controlled Synthesis)
“Size-Selective Encapsulation of C₆₀ by [10]Cycloparaphenylene: Formation of the Shortest Fullerene-Peapod”


– ICR Award for Graduate Students –
KOYAMA, Tomohiro (Nanospintronics)
“Observation of the Intrinsic Pinning of a Magnetic Domain Wall in a Ferromagnetic Nanowire”

POSTER PRESENTATIONS


 : Laboratory Whole Presentation
 : Laboratory Topic
 : General Presentation


— Organoelement Chemistry —


 “Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements”

 SAKAGAMI, Michiyasu; SASAMORI, Takahiro; TOKITOH, Norihiro
“Synthesis and Properties of Novel Bis(ferrocenyl)diphosphene Derivatives”


— Structural Organic Chemistry —


 “Research Activities in Structural Organic Chemistry Laboratory”

 NISHIMURA, Hidetaka; WAKAMIYA, Atsushi; MURATA, Yasujiro; FUKUSHIMA, Tatsuya; KAJI, Hironori
“Synthesis and Properties of Triphenylamine Derivatives with Quasi-Planar Structure”


 TANIGUCHI, Takuhiro; WAKAMIYA, Atsushi; MURATA, Yasujiro; DY, Joanne Ting; SEGAWA, Hiroshi
“Development of Organic Dyes for DSCs using Boryl-substituted Thienylthiazole as a Key Skeleton”


— Synthetic Organic Chemistry —

 TOMOHARA, Keisuke; YOSHIMURA, Tomoyuki; KAWABATA, Takeo
“Asymmetric α -arylation of α -amino Acids Derivatives”

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GE NAKANISHI, Koji; YAHATA, Yoshikazu; TSUJII, Yoshinobu; MORINAGA, Takashi; SATO, Takaya; YAMAGO, Shigeru
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GE YAHATA, Yoshikazu; NAKANISHI, Koji; KONISHI, Shota; YAMAGO, Shigeru; TSUJII, Yoshinobu
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GE NAKAMURA, Yasuyuki; ARIMA, Takahiro; TOMITA, Sora; YAMAGO, Shigeru
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GE YAMAMOTO, Kazutoshi; IMANISHI, Miki; FUTAKI, Shiroh
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GE IKEUCHI, Hideyuki; AHN, Yong-Mo; OTOKAWA, Takuya; WATANABE, Bunta; RICHARDS, G. J. Nigel; HIRATAKE, Jun
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Database Center for Life Science, Research Organization of
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Max Planck Gesellschaft, Marburg, Germany
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Center for Condensed Matter Sciences, National Taiwan University,
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Department of Chemistry, National Taiwan University, Taiwan
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Center for X-ray Optics, Lawrence Berkeley National Laboratory,
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Graduate School of Science, Hiroshima University, Hiroshima,
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Shanghai Institute of Organic Chemistry, China, P.R.
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Advanced Science Institute, RIKEN, Saitama, Japan
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Faculty of Life Sciences, Kyoto Sangyo University, Kyoto, Japan
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Department of Chemistry, University of Oregon, U.S.A.
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NCI-NIH, Laboratory of Receptor Biology and Gene Expression, U.S.A.
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Faculty of Engineering, Gifu University, Gifu, Japan
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- Prof NAGASHIMA, Hideo
Institute for Material Chemistry and Engineering, Kyusyu University, Fukuoka, Japan
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Max Planck Institute for Plant Breeding Research, Köln, Germany
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Faculty of Science, Hokkaido University, Hokkaido, Japan
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Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima, Japan
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Department of Applied Chemistry and Biotechnology, Okayama University of Science, Okayama, Japan
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Department of Chemistry, Uppsala University, Sweden
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Assist Prof SATO, Kengo
Department of Biosciences & Informatics-Faculty of Science and Technology, Keio University, Kanagawa, Japan
“Fast and Accurate Predictions of RNA Structures Using Integer Programming”
15 June 2011

Prof SCHWARZ, Helmut
Institut für Chemie, Technische Universität Berlin, Germany
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15 September 2011

Prof SEGI, Masahito
School of Chemistry, College of Science and Engineering, Kanazawa University, Kanazawa, Japan
“Efficient Construction of Selenium-containing Double Bonds and Application for Synthesis of Novel Heterocyclic Compounds”
10 June 2011

Prof SENTOKU, Yasuhiko
Department of Physics, University of Nevada, Reno, U.S.A.
“Enabling Numerical Modeling of Extreme-intensity Laser Produced Hot Dense Plasma”
6 July 2011

Assist Prof SUMIYAMA, Kenta
Division of Population Genetics, National Institute of Genetics, Mishima, Japan
“Understanding the Role of ‘Transcriptional Regulation Mechanisms Evolution’ on ‘Vertebrate Morphology Evolution’, through Mouse Transgenesis Analyses”
6 October 2011

Prof TAKADA, Shinji
Okazaki Institute for Integrative Bioscience, National Institute for Basic Biology, Aichi, Japan
“The Role of Fibronectin in the Morphogenesis of Vertebrate Embryos”
16 March 2011

Prof TANI, Keita
Department of Arts and Science, Osaka Kyoiku University, Osaka, Japan
“Development of Functional Carbazole Derivatives”
4 November 2011

Assist Prof TOMINAGA, Rumi
Interdisciplinary Research Organization, Miyazaki University, Miyazaki, Japan
“Analyses of MYB Transcription Factors that Regulate the Epidermal Cell Differentiation of *Arabidopsis thaliana*”
2 September 2011

Dr UCHIHASHI, Takashi
National Institute for Material Science, Japan
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20 October 2011

Prof UDAKA, Keiko
Department of Immunology, Kochi Medical School, Japan
“Development of a Peptide Immunotherapy for Malignant Tumors”
29 June 2011

Prof VARNEK, Alexandre
Laboratory of Chemoinformatics, University of Strasbourg, France
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Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China, P.R.
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Department of Chemistry, The University of Vermont, Vermont, U.S.A.
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Department of Physics, Faculty of Science, Naresuan University, Thailand
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Department of Chemistry, National University of Singapore, Singapore
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Organisch-Chemisches Institut, Westfälische Wilhelms-Universität,
Germany
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8 October 2011

Dr YAMADA, Yoichi
Advanced Science Institute, RIKEN, Saitama, Japan
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10 November 2011

Prof ZHOU, Huarong
The Chinese Academy of Sciences, Shanghai, China, P.R.
“Type 2 Diabetes, Is It an Intestinal Disease?”
13 September 2011

Dr ZIMMERMANN, Frank
CERN, Switzerland
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22 July 2011

MEETINGS AND SYMPOSIA

The 6th International Workshop for East Asian Young Rheologists
Contributed by WATANABE, Hiroshi as Co-Organizer
20–22 January 2011 (Yamagata, Japan)

**11th iCeMS International Symposium
“Chemical Control of Cells”**
Organized by UESUGI, Motonari
6 December 2011 (Kyoto, Japan)

KUBIC-NII Joint Seminar on Bioinformatics 2011
Organized by National Institute of Informatics and Institute for
Chemical Research
27 April 2011 (Kyoto, Japan)

1st Asia-Oceania Conference on Neutron Scattering
Co-organized by Asia-Oceania Association of Neutron Scattering,
Japanese Society for Neutron Science and ICR, and Other Facilities
(Conference Chair is KANAYA, Toshiji)
20–24 December 2011 (Tsukuba, Japan)

**GEOTRACES-Japan
“ICAS2011 Post Symposium”**
Organized by SOHRIN, Yoshiki
27 May 2011 (Uji, Japan)

Innovative Areas Symposium on “Hydration and ATP Energy”
Organized by SUZUKI, Makoto; KINOSHITA, Masahiro;
MATUBAYASI, Nobuyuki
9–11 August 2011 (Kyoto, Japan)

**ICR Symposium to Celebrate the Bioinformatics Center’s
10 Year Anniversary and New Restructuring**
Organized by AKUTSU, Tatsuya; MAMITSUKA, Hiroshi
Supported by Institute for Chemical Research
29 August 2011 (Kyoto, Japan)

**ICR-International Workshop
“International Workshop for Molecular Simulations for
Polymers”**
Organized by MASUBUCHI, Yuichi
9 September 2011 (Kyoto, Japan)

**The 2nd International Symposium on Multi-scale Simulations
of Biological and Soft Materials**
Contributed by MASUBUCHI, Yuichi as Co-Organizer
10–12 September 2011 (Kyoto, Japan)

**Biophysical Society Symposium on “Asymmetry Produced
by Water and ATP”**
Organized by SUZUKI, Makoto; MATUBAYASI, Nobuyuki
16–18 September 2011 (Himeji, Japan)

1st Meeting on Nano System for Young Scientists
Organized by NAMAZU, Takahiro; CHIBA, Daichi; NAGAO,
Yuuki; YOSHIDA, Hiroyuki
2 November 2011 (Uji, Japan)

The 8th Organoelement Chemistry Seminar
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro;
MIZUHATA, Yoshiyuki; AGOU, Tomohiro
21–22 November 2011 (Kyoto, Japan)

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