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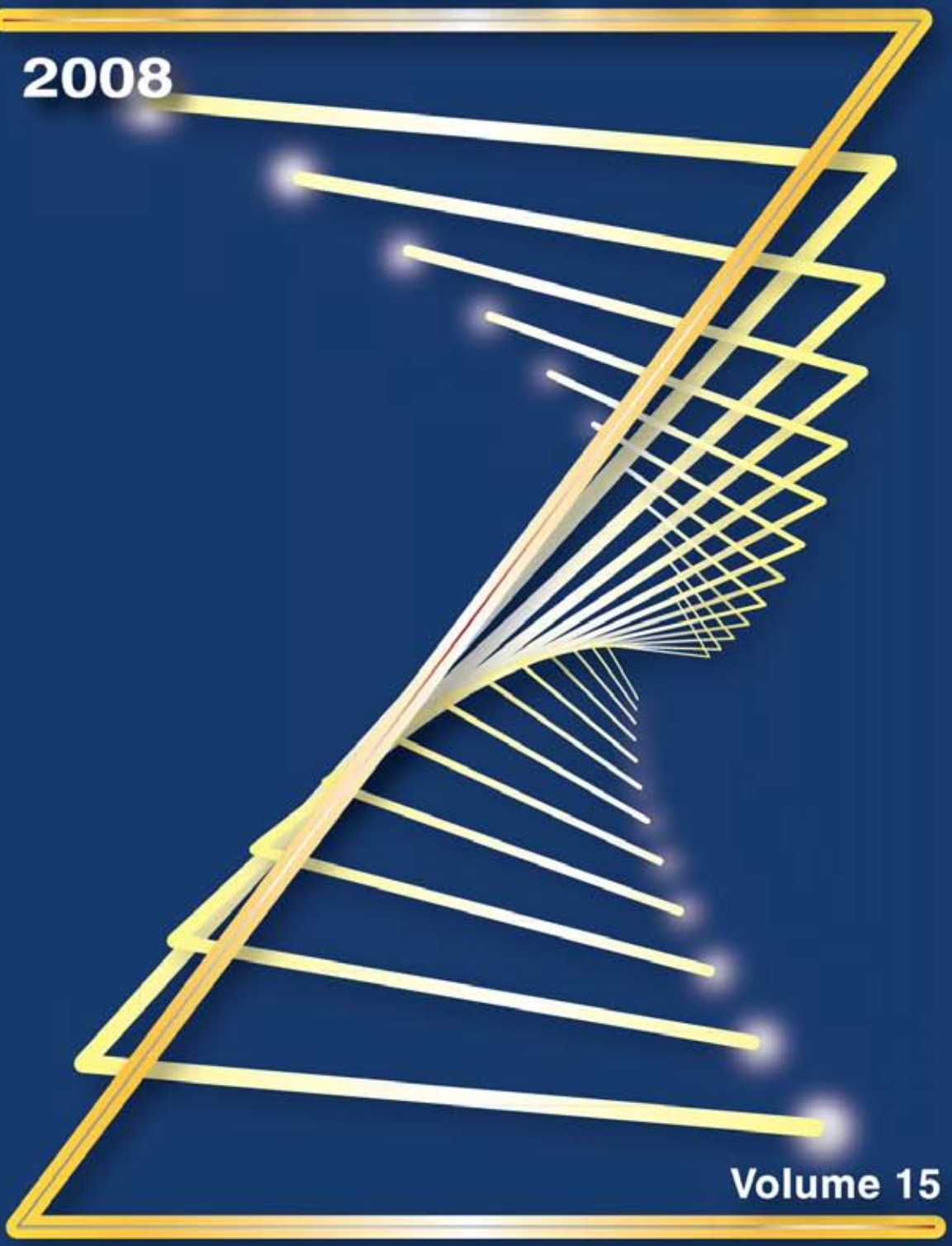
ICR ANNUAL REPORT

2008



Volume 15

Institute for Chemical Research
Kyoto University

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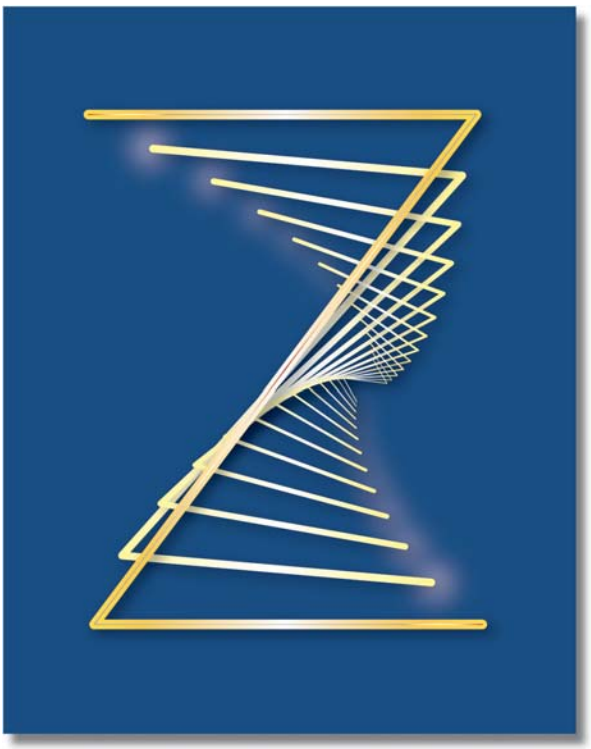
ICR ANNUAL REPORT 2008



Institute for Chemical Research
Kyoto University
Volume 15

Preface

Institute for Chemical Research (ICR) dates back to 1915 with the founding of the Specialized Center for Chemical Research 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. Although Japan was importing this drug, the outbreak of the World War I ceased the importation, and forced by circumstances the Japanese government requested that the University of Tokyo and Kyoto University 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, who had 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 is Japan's first synthetic fiber. Almost all the professors at the Institute, including the aforementioned, were also professors at the Faculty of Engineering or Science. However, over time, people began to recognize the importance of having professors dedicated solely to ICR in order to operate ICR with a clear responsibility, as well as the importance of the Institute's contribution in training researchers by providing guidance to graduate students. Thus, ICR began accepting graduate students in 1962, and reorganization in 1964 saw the installation of the research division system where each division was led by one of our dedicated professors.

Since the founding of ICR in 1926, our basic principle has been to excel in the investigation of the basic principles of chemistry and chemical applications. Through several reorganizations, 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 as well as the following three research centers: Advanced Research Center for Beam Science, International Research Center for Elements Science (IRCELS), and Bioinformatics Center.

Today, ICR spans 31 research fields (laboratories) with 104 faculty members and about 240 graduate students. Each laboratory belongs to one of the seven graduate schools, which encompass science, engineering, pharmaceutical sciences, agriculture, medicine, informatics, human and environmental studies. Our laboratories and the graduate schools work together to provide excellent graduate education.

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, ICR is multidimensional, and is constantly widening and deepening our research activities. We intend to use our strengths to contribute to pioneering research as well as to expand the boundaries of chemical related fields and to promote research collaborations, which are difficult using conventional graduate schools. Moreover, we aim to utilize our strengths as an outstanding research center in education in order to produce excellent scientists and engineers who possess a broad perspective and can positively contribute to our global society.

ICR is currently working towards establishing Global COE Programs in collaboration with the Graduate School of Engineering and the Graduate School of Science. In 2007, two programs have been selected from Kyoto University as Global COE Programs: International Center for Integrated Research and Advanced Education in Materials Science, which encompasses chemistry and materials science fields, and Center of Excellence for Education and Research on Photonics and Electronic Science and Engineering, which includes information science, electrical engineering, and electronics, and another Global COE: the Next Generation of Physics, Spun from Universality & Emergence, have started in 2008. In addition, ICR is making enthusiastic contribution to the "Joint Project of Chemical Synthesis Core Research Institutions (2005–2010)", developed by IRCELS (ICR) at Kyoto University in collaboration with the Research Center for Materials Science at Nagoya University and the Institute for Materials Chemistry and Engineering at Kyushu University. This project is supported by MEXT through the Research and Education Funding for Inter-University Research Project. We, at the Institute for Chemical Research, would like to be a focal point in the Centers of Excellence by gathering chemists in our three campuses at Yoshida, Uji, and Katsura, and by serving as a bridge between science and engineering. Thus, we respectfully request your continued support and encouragement.

January 2009

TOKITOH, Norihiro
Director

ICR News 2008

Activity Report of the Global COE Programs

"International Center for Integrated Research and Advanced Education in Materials Science"

Representative from ICR:

Prof TOKITOH, Norihiro (Director of ICR)

Division of Synthetic Chemistry
—Organoelement Chemistry—

→P.4

The Project, granted in the area "Chemistry and Materials Science" for fiscal 2007–2011, is intended to consolidate the over 100 chemistry-related research groups of Kyoto University in Graduate School of Engineering, Graduate School of Science, and Institute for Chemical Research (ICR), covering virtually all the arenas of chemistry from basic to engineering and from molecules to materials, for the ultimate goal of "Integrated Materials Science."

The main two objectives of this Project are (1) Program in Research: International Center for Integrated Materials Science and (2) Program in Education: A New Breed of Internationally Competent Young Scientists, and we are now fowarding with a variety of sub-projects as follows (the numbers are those for ICR).

1) Inter-Field Joint Research Projects (Integration beyond Core Fields)
2) Interfaculty Integrated Course Program
3) Embryonic Research Project Support (FY2007: 10 Assistant Professors and 9 Students, FY2008: 10 Assistant Professors and 9 Students)
4) International Academic Exchange Program: On-the-research Training beyond Borders (FY2007: 3 Assistant Professors, 1 PD and 9 Students, FY2008: 1 Assistant Professors and 10 Students)
5) GCOE Post-doctoral fellows and Research Assistants (FY2007: 1 PD and 33 RAs, FY2008: 4 PDs and 33 RAs)
6) International Scholarship (FY2007: 7 GCOE-Seminars and Lectureships, FY2008: 9 GCOE Seminars and Lectureships)
7) Foreign Graduate Student Internship (FY2007: 0 persons, FY2008: 1 persons)
8) International Workshop Initiative (FY2007: 1 events, FY2008: 2 events)

As for the International Academic Exchange Program, in particular, many applications have been made from a variety of research groups in ICR and the qualified young chemits have enjoyed their flexible, short-stay studies abroad (varying from two weeks through three months). Other projects have also been progressed smoothly.

In interdisciplinary collaboration and perhaps in fusion with physics and biology, chemistry and materials science today are thus expected to make fundamental contribution to science per se and to the global society beyond tomorrow. All the members of the COE Project are sincerely determined to create the new paradigm of "Integrated Materials Science" and thereby to cultivate new breeds of young scientists, truly competent, creative, and energetic, who will soon take off from Kyoto University towards international arenas of science and beyond.

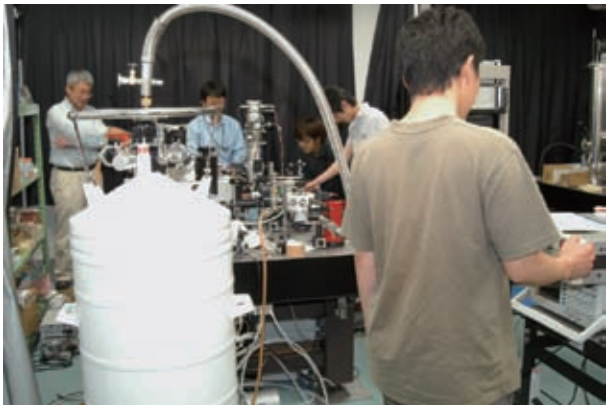
"Center of Excellence for Education and Research on Photonics and Electronics Science and Engineering"

Representative from ICR:

Prof KANEMITSU, Yoshihiko

International Research Center for Elements Science
—Photonic Elements Science— →P.56

In this program, we aim at establishing the COE for "photonics and electronics science and engineering", to investigate and develop innovative technologies, by which an arbitrary manipulation of photons (light) and an ultimate control of electrons will be achieved, as we hold the motto of "challenge the limitations of current technology and create new functionalities". In this year, we organized the international conference for young researchers and students and the seminar school for students "dojyo". Two ICR students visited several Universities and Research Institutes in Europe in this summer.



"The Next Generation of Physics, Spun from Universality & Emergence —Developing Independent Researchers to Explore New Frontiers—"

The program of the Global Centers of Excellence (GCOE), funded by the Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT), is organized by the members of the Division of Physics and Astronomy and its joint courses (the Kwasan and Hida Observatories, the Yukawa Institute for Theoretical Physics, the Institute for Chemical Research, and the Research Center for Low Temperature and Materials Sciences). From the ICR, the courses of Particle Beam Science, Laser Matter Interaction Science, and Atomic and Molecular Physics in the Advanced Research Center for Beam Science join this program.

The natural world to whose investigation we are dedicated consists of phenomena on unfathomably varying scales from elementary particles and atomic nuclei to the macroscopic world of living organisms and our earth to the great variety of phenomena and physical laws that appear as qualitatively differing strata of nature. Corresponding to these individual strata there are separate fields of research, each possessing its own sets of concepts and theories.

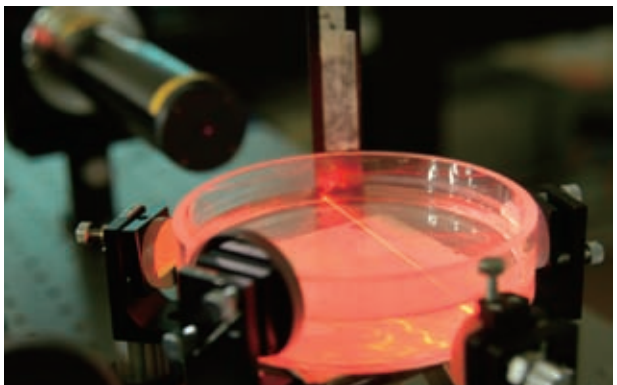
In this Global COE, we seek to unite these seemingly independent realms by uncovering the fundamental universality extending across their boundaries, while searching for novel and diverse emergent phenomena that could not be predicted by deduction from such laws alone. The objective of the proposed GCOE is to make progress toward the construction of the next generation of physics, spun from universality and emergence, while developing independent-minded researchers who will be capable of opening new frontiers in the study of natural phenomena.

http://www.scphys.kyoto-u.ac.jp/gcoe/index_e.html

Representative from ICR:

Prof SAKABE, Shuji

Advanced Research Center for Beam Science
—Laser Matter Interaction Science— →P.44

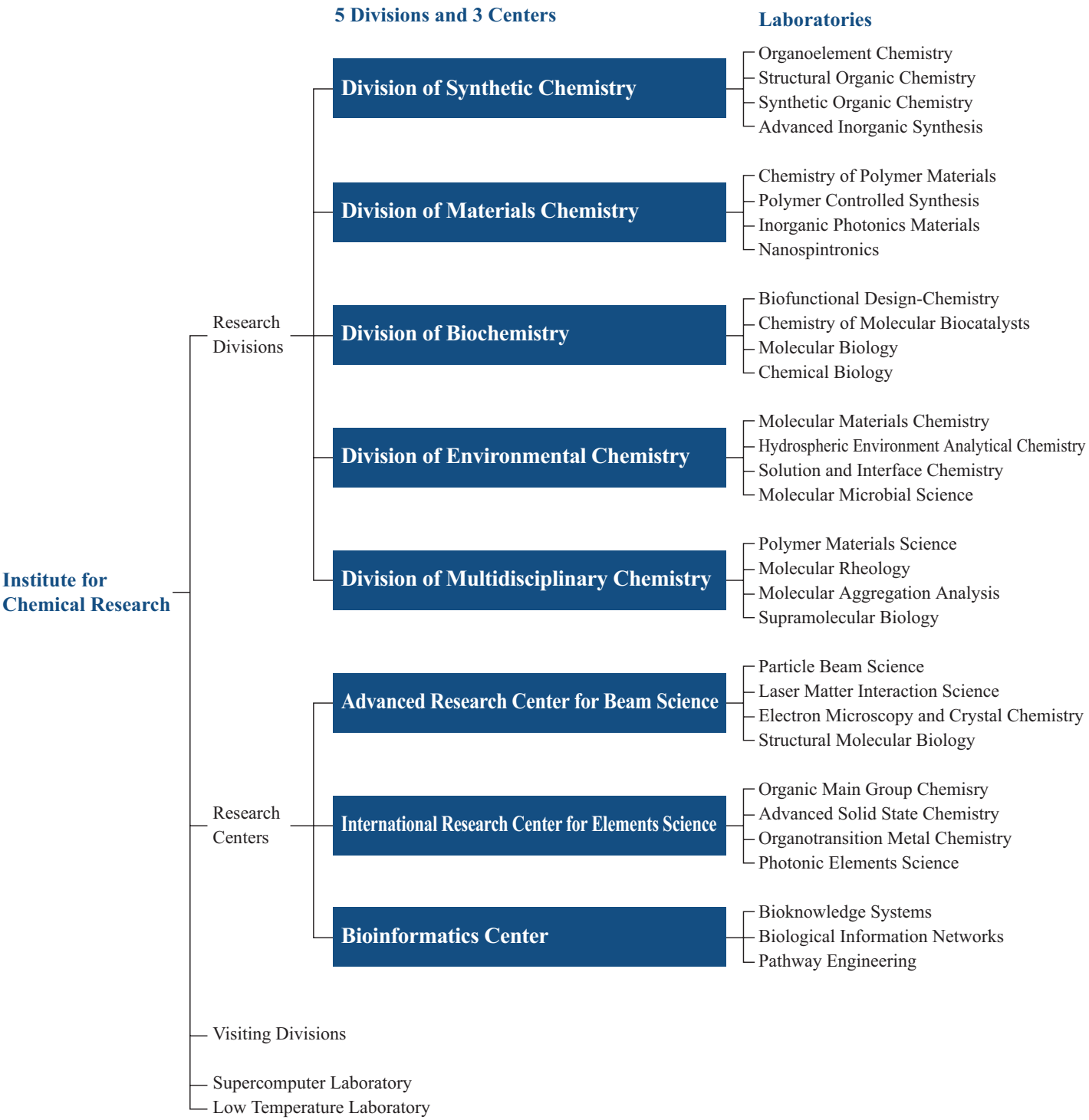


CONTENTS

Abbreviations used in the columns

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

ORGANIZATION


5 Divisions and 3 Centers
Laboratories
Institute for Chemical Research
Research Divisions
Division of Synthetic Chemistry
Organoelement Chemistry
Structural Organic Chemistry
Synthetic Organic Chemistry
Advanced Inorganic Synthesis
Division of Materials Chemistry
Chemistry of Polymer Materials
Polymer Controlled Synthesis
Inorganic Photonics Materials
Nanospintronics
Division of Biochemistry
Biofunctional Design-Chemistry
Chemistry of Molecular Biocatalysts
Molecular Biology
Chemical Biology
Division of Environmental Chemistry
Molecular Materials Chemistry
Hydrospheric Environment Analytical Chemistry
Solution and Interface Chemistry
Molecular Microbial Science
Division of Multidisciplinary Chemistry
Polymer Materials Science
Molecular Rheology
Molecular Aggregation Analysis
Supramolecular Biology
Research Centers
Advanced Research Center for Beam Science
Particle Beam Science
Laser Matter Interaction Science
Electron Microscopy and Crystal Chemistry
Structural Molecular Biology
International Research Center for Elements Science
Organic Main Group Chemisry
Advanced Solid State Chemistry
Organotransition Metal Chemistry
Photonic Elements Science
Bioinformatics Center
Bioknowledge Systems
Biological Information Networks
Pathway Engineering
Visiting Divisions
Supercomputer Laboratory
Low Temperature Laboratory

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry
- Organoelement Chemistry -

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

Prof
TOKITOH, Norihiro
(D Sc)

Assoc Prof
NAKAMURA, Kaoru
(D Sc)

Assist Prof
SASAMORI, Takahiro
(D Sc)

Assist Prof
MIZUHATA, Yoshiyuki
(D Sc)

Techn
HIRANO, Toshiko

Proj Res*
NAGAHORA, Noriyoshi
(D Eng)

Proj Res**
TAJIMA, Tomoyuki
(D Sc)

PD
OPPERMANN, Gerrit
(Ph D)

PD
MORIKAWA, Satoshi
(D Eng)

*Assist Prof (SER) of Institute of Sustainability Science

** Assist Prof of Pioneering Research Unit for Next Generation

Students

KAWAI, Masahiro (D3)
OZAKI, Shuhei (D3)
TANABE, Taro (D3)
YUASA, Akihiro (D3)
INAMURA, Koji (D2)
MATSUMOTO, Teruyuki (D2)
TANABE, Yusuke (D2)
TSURUSAKI, Akihiro (D2)
MIEDA, Eiko (D1)
KANEKO, Yoshikazu (M2)
SATO, Takahiro (M2)
YAMAMOTO, Osami (M2)
SAKAI, Kiyomichi (M1)
NIWA, Masatoshi (M1)

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 reactivity 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. Organic synthesis mediated by biocatalysts is also studied.

Research Activities (Year 2008)

Publications

Sasamori T, Hironaka K, Sugiyama Y, Takagi N, Nagase S, Hosoi Y, Furukawa Y, Tokitoh N: Synthesis and Reactions of a Stable 1,2-Diaryl-1,2-dibromodisilene: A Precursor for Substituted Disilenes and a 1,2-Diaryldisilyne, *J. Am. Chem. Soc.*, **130**, 13856-13857 (2008).

Sasamori T, Yuasa A, Hosoi Y, Furukawa Y, Tokitoh N: 1,2-Bisferrocenyldisilene: A Multi-step Redox System with an Si=Si Double Bond, *Organometallics*, **27**, 3325-3327 (2008).

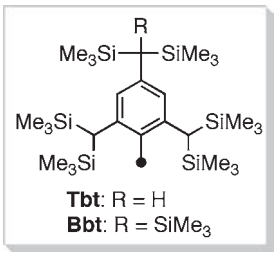
Tanabe T, Mizuhata Y, Takeda N, Tokitoh N: Syntheses and Structures of Platinum Siloxides Bridged by a Sulfur or Selenium Atom and a Unique 1,3-Aryl Migration from Silicon to Platinum through the Si–O–Pt Linkages, *Organometallics*, **27**, 2156-2158 (2008).

Presentations

Synthesis and Properties of Stable 2-Metallanaphthalenes of Heavier Group 14 Elements, Mizuhata Y, Sasamori T, Nagahora N, Watanabe Y, Furukawa Y, Tokitoh N, Dalton Discussion 11: The Renaissance of Main Group Chemistry, University of California, Berkeley, USA, 24 June 2008 (invited).

Redox Behavior and Coordination Chemistry of Kinetically Stabilized Silaaromatics and Related Compounds, Matsumoto Ta, Tanabe Y, Mizuhata Y, Sasamori S,

Synthesis of a Novel Silicon–Silicon Triple-Bond Compound



There has been much interest in the chemistry of multiply bonded organosilicon compounds, *i.e.*, disilenes (>Si=Si<) and disilynes (–Si≡Si–). While a lot of kinetically stabilized disilenes have been synthesized and characterized, only two examples of stable disilynes bearing bulky silyl groups have been known up to now. We have reported the synthesis and structure of the first stable 1,2-diaryldisilyne by taking advantage of Bbt groups. The diaryldisilyne has a crystallographic *C*2 axis through the central Si≡Si bond (Figure 1). Its Si≡Si bond length [2.108(5) Å] is reasonably shorter than the typical Si–Si and Si=Si bond lengths, featuring its triple-bond character.

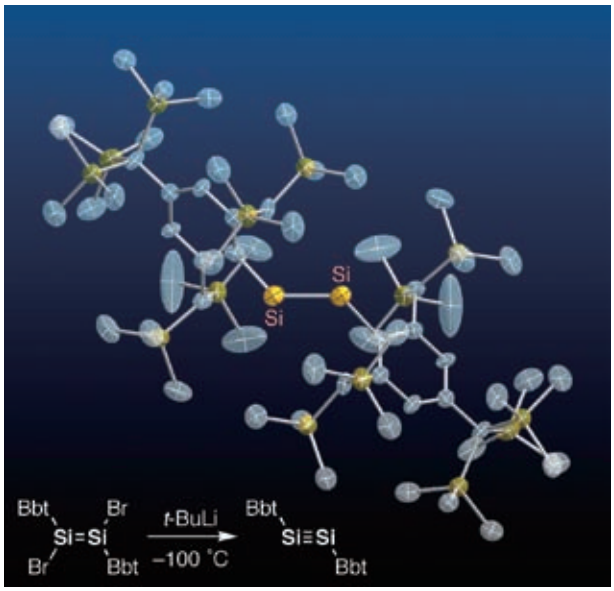


Figure 1. Synthesis and Structure of Disilyne (–Si≡Si–).

1,3-Aryl Migration from Silicon to Platinum

We have found that platinum siloxides **1** underwent a unique 1,3-migration of the Mes (2,4,6-trimethylphenyl) group from the silicon atom to the platinum center on treatment with chloride ion in the presence of a Brønsted acid, affording the corresponding complexes **2** in moderate yields (Figure 2). It should be noted that the 1,3-migration reactions described here are very important, as they provide the first experimental demonstration of the transmetalation of a carbon substituent from a silicon atom to a transition metal center in a metal siloxide, the process of which is postulated as a plausible mechanism for some silicon-containing catalytic systems, such as the palladium(0) catalyzed cross-coupling reaction of aryl- or alkenylsilanols with aryl or vinyl iodides in the presence of tetrabutylammonium fluoride.

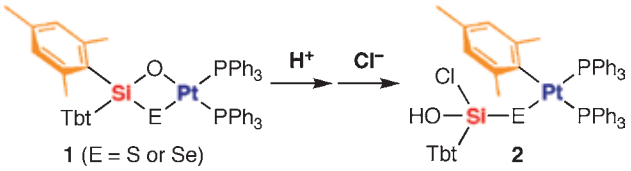


Figure 2. 1,3-Mesityl Migration Reaction.

Tokitoh N, The 15th International Symposium on Organosilicon Chemistry, Jeju, Korea, 2 June 2008 (invited).

New Aspects in the Chemistry of Doubly Bonded Systems between Heavier Group 15 Elements, Tokitoh N, Heterocyclic and Heteroatom Chemistry Conference 2008, Cancun, Mexico, 25 Feburary 2008 (invited).

Grants

Tokitoh N, Sasamori T, Nagahora N, Mizuhata Y, The Chemistry of Unsaturated Compounds of Heavier Main Group Elements: Pursuit of Novel Properties and Functions, Grant-in-Aid for Creative Scientific Research, 1 April 2005–31 March 2010.

Sasamori T, Construction of Novel Extended π-Electron Conjugated Systems Containing Heavier Main Group Elements, Grant-in-Aid for Young Scientists (B), 1 April 2006–31 March 2008.

Sasamori T, Construction of Novel d-π Electron Conjugated Systems Containing Heavier Main Group Elements and Transition Metals and Elucidation of Their Properties. Grant-in-Aid for Science Research on Priority Areas "Synergy of Elements", 1 April 2007–31 March 2010.

Nagahora N, Study on Development of Novel Molecular Devices Bearing Metallocene and Double Bonds between Heavier Group 15 Elements, Kinki Invention Center, 1 April 2007–31 March 2008.

Awards

Tanabe T, The Best Poster Award, The 2nd Asian Silicon Symposium, 6 June 2008.

Mizuhata Y, Mitsubishi Kagaku Award in Synthetic Organic Chemistry, Japan, 20 February 2008.

Division of Synthetic Chemistry
- Structural Organic Chemistry -

http://hydrogen.kuicr.kyoto-u.ac.jp/K_eHP_F/main.html

Assoc Prof
MURATA, Yasujiro
(D Eng)

Assist Prof
MURATA, Michihisa
(D Eng)

PD
KUROTOBI, Kei
(D Sc)

Students

KATO, Keisuke (M2)
MORINAKA, Yuta (M1)
HIROSE, Yuya (UG)

Visitor

Mr JOHNSON, Jeremiah Columbia University, USA, 6 June–22 July 2008

Scope of Research

Fundamental studies are being conducted for creation of new functional π-systems with novel structures and properties. 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 π-systems with curved structure.

Research Activities (Year 2008)

Publications

Murata M, Ochi Y, Tanabe F, Komatsu K, Murata Y: Internal Magnetic Fields of Dianions of Fullerene C_{60} and Its Cage-Opened Derivatives Studied by Encapsulated H_2 as an NMR Probe, *Angew. Chem. Int. Ed.*, **47**, 2039-2041 (2008).

Murata Y, Maeda S, Murata M, Komatsu K: Encapsulation and Dynamic Behavior of Two H_2 Molecules in an Open-Cage C_{70}, *J. Am. Chem. Soc.*, **130**, 6702-6703 (2008).

Murata M, Maeda S, Morinaka Y, Murata Y, Komatsu K: Synthesis and Reaction of Fullerene C_{70} Encapsulating Two Molecules of H_2, *J. Am. Chem. Soc.*, **130**, 15800-15801 (2008).

Presentations

Synthesis of Endohedral Open-Cage Fullerenes and Studies on Non-Covalent Interaction between Encapsulated Species and Fullerene Cage, Murata Y, Cuang S-C, Murata M, Komatsu K, 213th ECS Meeting, 19 May 2008, Phoenix, USA (invited).

Organic Synthesis of Endohedral Fullerenes, Murata Y, Symposium on H_2@C_{60}, 15 August 2008, New York, USA (invited).

Synthesis and Properties of Novel Open-Cage Fullerene Derivatives, Kurotobi K, Murata M, Murata Y, PRiME 2008, 12 October 2008, Honolulu, USA.

Generation of Ionic [60] Fullerene Derivatives Encapsulating Molecular Hydrogen, Murata M, Ochi Y, Tanabe F, Murata Y, Komatsu K, PRiME 2008, 13 October 2008, Honolulu, USA.

Grants

Murata Y, PRESTO, Japan Science and Technology Agency, October 2005–March 2009.

Murata Y, Grant-in-Aid for Scientific Research on Priority Areas, "Molecular Theory for Real Systems", April 2007–March 2009.

Murata M, Grant-in-Aid for Young Scientists (B), April 2007–March 2009.

Murata Y, Grant-in-Aid for Young Scientists (A), April 2008–March 2011.

Murata Y, Grant-in-Aid for Scientific Research on Innovative Areas, December 2009–March 2014.

Encapsulated H_2 Molecule as an NMR Probe

Magnetic properties of inside of fullerenes are very interesting because ring current effects of three-dimensional π-system of fullerenes are reflected critically. We measured ^{1}H NMR chemical shifts of molecular hydrogen encapsulated in dichloromethyl-C_{60} cation and (1-octynyl)-C_{60} anion in order to clarify the difference in magnetic shielding effects inside the fullerene cages. The signals of the H_2 molecule inside both cationic and anionic C_{60} cages appeared in lower fields as compared to those of neutral counterparts. In contrast, upon ^{1}H NMR measurement of $H_2@C_{60}^{2-}$, a signal of the encapsulated H_2 appeared at extraordinarily low magnetic field such as δ = +26.36 ppm in acetonitrile-d_3. According to the results of NICS calculations for $H_2@C_{60}^{2-}$, magnetic properties of hexagons and pentagons on C_{60} were shown to be totally reversed as compared to those of neutral C_{60}.

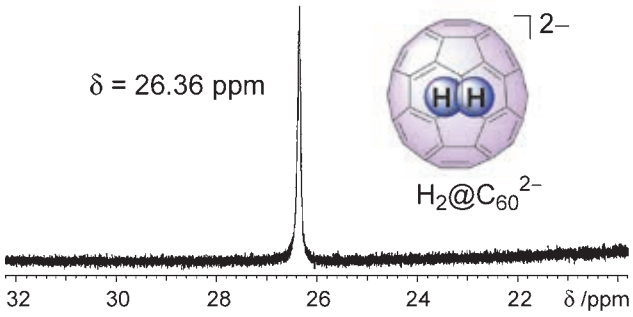


Figure 1. ^{1}H NMR spectrum (300 MHz, CD_3CN) of $H_2@C_{60}^{2-}$.

Encapsulation and Dynamic Behavior of Two H_2 Molecules in an Open-Cage C_{70}

Encapsulation of small molecules in a small space with sub-nanometer size are currently attracting wide interests from the view point of basic science as well as storage purpose. Open-cage fullerenes are one of the ideal systems with a hollow space inside the carbon cage. In contrast with open-cage C_{60}, examples of open-cage C_{70} are quite limited. Recently, we synthesized an open-cage C_{70} derivative, which has an opening large enough for hydrogen molecule to pass through. Under the high pressure of hydrogen, this open-cage C_{70} encapsulated not only one H_2 molecule but also two H_2 molecules reflecting the larger inner space than C_{60}. The two H_2 molecules trapped inside the open-cage C_{70} showed a rapid exchange of their relative positions as observed by the ^{1}H NMR measurement at room temperature. This exchange slowed down at low temperature. The ^{1}H NMR at –100 °C clearly showed two sharp signals corresponding to two individual H_2 molecules encapsulated in the open-cage C_{70}. This is the first example of observing the dynamic behavior of two hydrogen molecules in a tightly confined space.

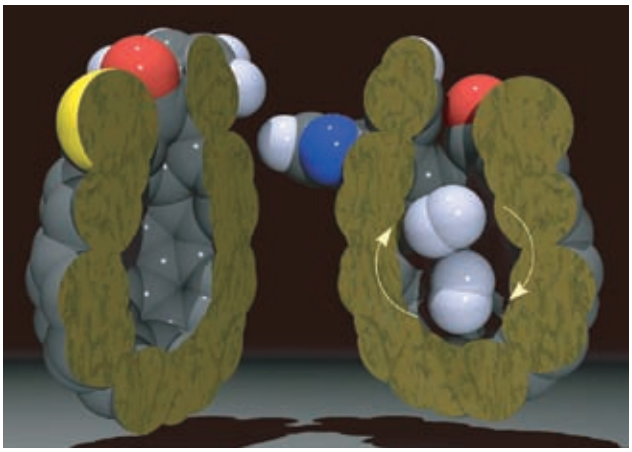


Figure 2. Cut-out view of open-cage C_{70} derivative encapsulating two molecules of hydrogen.

Synthesis and Reaction of $H_2@C_{70}$ and $(H_2)_2@C_{70}$

We have previously established a methodology to realize endohedral fullerene C_{60} containing one molecule of H_2 by organic synthesis, so-called "molecular surgery". In the present research, the scope of the molecular surgery method is extended to the representative higher fullerene, C_{70}, to provide a novel endohedral fullerene C_{70} encapsulating one and two molecules of H_2 from their open-cage derivatives. Actually, $H_2@C_{70}$ and $(H_2)_2@C_{70}$ were synthesized and characterized. For the clarification of difference in reactivity between $H_2@C_{70}$ and $(H_2)_2@C_{70}$, the equilibrium constants for the Diels-Alder reaction of $H_2@C_{70}$ and $(H_2)_2@C_{70}$ with 9,10-dimethylanthracene (DMA) have been determined at 30, 40, and 50 °C. The decreased equilibrium constants of $(H_2)_2@C_{70}$ to the addition of DMA as compared to that of $H_2@C_{70}$ has been demonstrated.

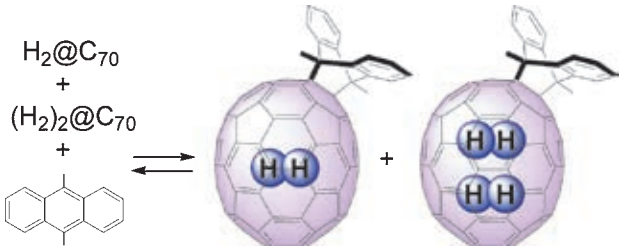


Figure 3. Reaction of $H_2@C_{70}$ and $(H_2)_2@C_{70}$ with 9,10-Dimethylanthracene.

Division of Synthetic Chemistry
- Synthetic Organic Chemistry -

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

Prof
KAWABATA, Takeo
(D Pharm Sc)

Assoc Prof
FURUTA, Takumi
(D Pharm Sc)

Assist Prof
YOSHIMURA, Tomoyuki
(D Pharm Sc)

Techn
TERADA, Tomoko

PD
SOKEIRIK, Yasser Samir
Abdel-khalek
(D Pharm Sc)

Students

KAN, Keizo (D3)
WATANABE, Toshihide (D3)
IRIE, Kazuyuki (D2)
URUNO, Yoshiharu (D2)
HAYASHI, Kazuhiro (D1)
SUE, Daisuke (D1)
YOSHIDA, Keisuke (D1)
YAMAMOTO, Junya (D1)
IMAMURA, Yoko (M2)
TOMOHARA, Keisuke (M2)
MISHIRO, Kenji (M1)
SAKAI, Hiroki (M1)
TAKUWA, Masatoshi (M1)
UEDA, Yoshihiro (M1)

Visitors

Prof ZIPSE, Hendrik — Ludwig-Maximilians-Universität in München, Germany, 9 September 2008
Prof WORTH, Thomas — Cardiff University, UK, 26 September 2008

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", nucleophilic catalysis for fine organic syntheses, synthesis of unusual amino acids and nitrogen heterocycles, regioselective functionalization of carbohydrates, visualization of molecular information by functional phenolphthaleins, synthesis and properties of homochiral oligonaphthalenes, and the structural and functional investigation of heterochiral oligomers.

Research Activities (Year 2008)

Publication

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).

Presentations

Asymmetric Reactions with Axially Chiral Compounds, Symposium on Molecular Chirality 2008, Kawabata T, 23 May 2008.

Asymmetric Synthesis *via* Planar Chiral Enolates, Third International Conference on Advanced Organic Synthesis Directed toward the Ultimate Efficiency and Practicability, Yoshimura T, 27 May 2008.

Convenient Synthesis of Axially Chiral Biaryls via a Pd-Catalyzed Domino Coupling Reaction, 17th International Conference on Organic Synthesis (ICOS-17), Furuta T, 24 June 2008.

Toward the Development of Intelligent Catalysts: Catalyst Design Based on Dynamic Molecular Recognition, Seminar of The Society of Synthetic Organic Chemistry, Japan, Tokai-Branch, Kawabata T, 12 July 2008.

Selective Acylation by Intelligent Nucleophilic Catalysis, UK/Japan Symposium on Asymmetric Catalysis, Kawabata T, 9 December 2008.

Acylation Catalysis via Fine Molecular Recognition, The Forth Symposium on Functional Molecules, Kawabata T, 20 December 2008.

Grants

Kawabata T, Fine Organic Synthesis by Nucleophilic Catalysis, Grant-in Aid for Scientific Research (A), 1 April 2006–31 March 2009.

Kawabata T, Advanced Molecular Transformation with Functional Carbanions, Grant-in Aid for Scientific Research on Priority Areas, 1 October 2005–31 March 2009.

Kawabata T, Creation of Novel Binaphthyls with Inner Hydrogen Bonding, Grant-in-Aid for Exploratory Research,

Asymmetric Synthesis via C-O Axially Chiral Enolates

Enantioselective construction of tetrasubstituted carbon has been the focus of current synthetic attention. We have developed a method for enantioselective construction of cyclic ethers with tetrasubstituted carbon via C-O axially chiral enolates for the first time. Treatment of chiral aryl alkyl ethers **1** derived from readily available cheap lactic acid with a base gave chiral dihydrobenzofurans **2**. Effects of substituent R in **1** were critical on asymmetric induction. Treatment of **1** (R=Me) with sodium hexamethyldisilazide (NaHMDS) at −78 °C gave cyclization product **2** (R=H) as a racemate, while that of **1** (R=Me) or **1** (R=^{i}Pr) gave **2** (R=Me) or **2** (R=^{i}Pr) in 84% ee or 99% ee, respectively. Racemization barrier of the planar chiral enolate (R=^{i}Pr) was estimated to be ~11.5 kcal/mol by variable-temperature NMR measurement of the corresponding *tert*-butyldimethylsilyl ether. Based on the barrier, the half-life of racemization of the planar chiral enolate was roughly calculated to be ~1 second at −78 °C. Thus, asymmetric synthesis via intrinsically chiral enolates with very short half-lives of racemization has been achieved.

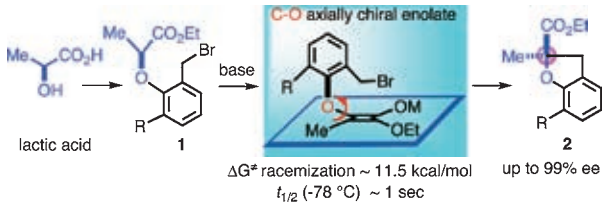


Figure 1.

Powdered KOH in DMSO: An Efficient Base for Asymmetric Cyclization at Ambient Temperature

Enolate chemistry has been extensively used for stereoselective C-C bond formation, in which metal amide bases are frequently employed in strictly anhydrous solvents at low temperatures. However, we found that asymmetric intramolecular C-C bond formation via axially chiral enolate intermediates proceeded in up to 99% ee at 20 °C by using powdered KOH in dry or wet DMSO as a base. The enantioselectivity was even higher than that of the corresponding reactions with potassium hexamethyldisilazide in DMF at −60 °C. The racemization barrier of the axially chiral enolate intermediate was experimentally estimated to be ~15.5 kcal/mol. Based on the barrier, the chiral enolate intermediate was supposed to undergo cyclization within ~10^{-3} sec at 20 °C after it is generated to give the product in ≥99% ee. The rate-determining step for the cyclization must be the enolate-formation step because the half-lives of racemization of the chiral enolate intermediates generated from **3** are supposed to be much shorter (< 0.1 sec) than the time required for the reactions to be complete (2~12 h). Thus, C-N axially chiral enolates would form gradually, and once formed, would immediately undergo asymmetric cyclization due to their extremely high reactivity.

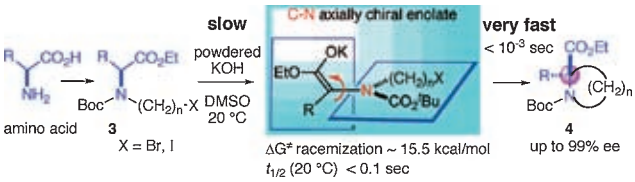


Figure 2.

Construction of Axially Chiral Amino Acids via Pd-Mediated Synthesis of Azahelicenes

Unnatural amino acids have attracted considerable attention in the field of asymmetric synthesis as well as medicinal chemistry. Although unnatural amino acids with central chirality have been well developed, axially chiral amino acids have not yet been well exploited. We have developed a straightforward method for the construction of axially chiral amino acids via Pd-mediated synthesis of azahelicenes. Domino coupling reactions of **4** proceeded in the presence of catalytic amount of $Pd_2(dba)_3$ without additional ligands to afford azahelicenes **5** via successive C–C (red colored) and C–N (green colored) bond formations. The amide bond of **5** was cleaved under basic conditions to afford novel axially chiral amino acids **6**, which possesses amino and carboxyl groups at C-2 and C-2' positions, respectively.

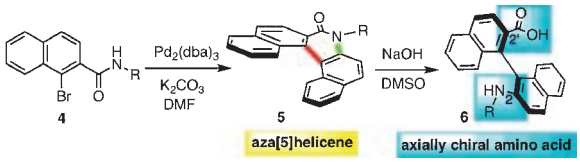


Figure 3.

1 April 2007–31 March 2009.

Furuta T, Synthesis of Functionalized Artificial Phospholipids for Investigation of Membrane Related Biosystems, Grant-in-Aid for Scientific Research (C), 1 April 2008–31 March 2011.

Yoshimura T, Syntheses of Natural Products via Memory of Chirality, Grant-in-aid for Young Scientists (B), 1 April 2007–31 March 2009.

Division of Materials Chemistry
- Chemistry of Polymer Materials -

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

Prof
TSUJII, Yoshinobu
(D Eng)

Assist Prof
OHNO, Kohji
(D Eng)

Assist Prof
GOTO, Atsushi
(D Eng)

PD
KIM, Jeong Sik
(D Eng)

Proj Res
SHINJO, Ayaka

Students

OKAYASU, Kenji (D3)
NOMURA, Akihiro (D1)
KAYAMA, Yuzo (M2)
NAGASAWA, Koji (M2)
YOSHIOKA, Yuu (M2)
AKASHI, Tatsuki (M1)
HSU, Sho Yao (M1)
HUANG, Yun (RS)
NAKAHARA, Ryo (UG)
TAKATA, Akisato (UG)
SHINMURA, Masahito (UG)

Visitors

Prof WATANABE, Junji	Tokyo Institute of Technology, 4 April 2008
Mr BOMPART, Mark	Compiegne University of Technology, France, 24 June–19 August 2008
Prof HAUPT, Karsten	Compiegne University of Technology, France, 6 September 2008
Prof KITAOKA, Takuya	Kyushu University, 18 December 2008
Prof FUJIKAWA, Seizo	Hokkaido Univesity, 19 December 2008

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).

Research Activities (Year 2008)

Publications

Arita T, Kayama Y, Ohno K, Tsujii Y, Fukuda T: High-Pressure Atom Transfer Radical Polymerization of Methyl Methacrylate for Well-Defined Ultrahigh Molecular-Weight Polymers, *Polymer*, **49**, 2426-2429 (2008).

Morinaga T, Ohno K, Tsujii Y, Fukuda T: Structural Analysis of Semisoft Colloidal Crystal by Confocal Laser Scanning Microscopy, *Macromolecules*, **41**, 3620-3626 (2008).

Goto A, Tsujii Y, Fukuda T: Reversible Chain Transfer Catalyzed Polymerization (RTCP): A New Class of Living Radical Polymerization, *Polymer*, **49**, 5177-5184 (2008) (Feature Article).

Presentations

Tsujii Y, Novel Properties of CPBs. Int. Conf. Adv. Func. Polym. Self-Org. Mater. (IC-PSM 2008), Busan, Korea, 22–26 September 2008.

8 Presentations, 57th Spring Meeting, Soc. Polym. Sci., Jpn., Yokohama, 28–30 May 2008.

5 Presentations, 57th Autumn Meeting, Soc. Polym. Sci., Jpn., Osaka, 24–26 September 2008.

Grants

Fukuda T, Science and Technology of CPB, Grant-in-Aid for Specially Promoted Research, 1 April 2005–31 March 2009.

Tsujii Y, Creation of New Bio-Interfaces Based on CPB, Grant-in-Aid for Science Research (A), 1 April 2005–31 March 2008.

Tsujii Y, Development of Novel Lithium Ion Battery with Network Channel of High Ionic-Conductivity,

High-Pressure Atom Transfer Radical Polymerization of Methyl Methacrylate for Well-Defined Ultrahigh Molecular-Weight Polymers

The feasibility of high-pressure atom transfer radical polymerization (ATRP) for synthesizing well-defined polymers of extraordinarily high molecular weights was demonstrated. ATRP of methyl methacrylate (MMA) under pressures up to 500 MPa was investigated at 60°C. The addition of a small amount of a $Cu(II)Cl_2$/ligand complex along with the general benefits of high pressure of enhancing propagation and suppressing termination brought about an excellent control of polymerization even with an extremely low concentration of ATRP initiator. For example, there was produced PMMA with a number-average molecular weight M_n of 3.6×10^6 and a polydispersity index (M_w/M_n) of 1.24, which has never been achieved by conventional ATRP.

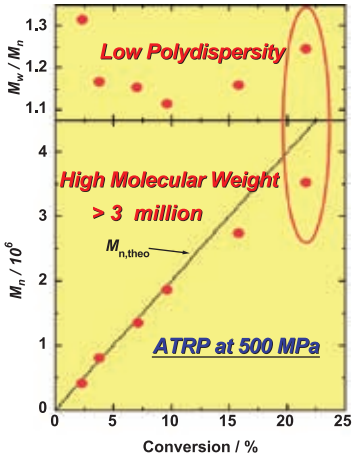


Figure 1. Plot of M_n and M_w/M_n vs monomer conversion for the ATRP of MMA at 500 MPa.

Alcohols as a Novel Class of Catalysts for a Living Radical Polymerization

Alcohols (phenols and a vinyl alcohol) were successfully used as a novel class of catalysts for a living radical polymerization (RTCP). Low-polydispersity polystyrenes and polymethacrylates with predicted molecular weight were obtained with a fairly high conversion in a fairly short time. Notably, the alcohols include common antioxidants for foods and resins (e.g., BHT), phenol itself, and even natural compounds (e.g., vitamins). Their commonness and environmental safety may be attractive for practical applications.

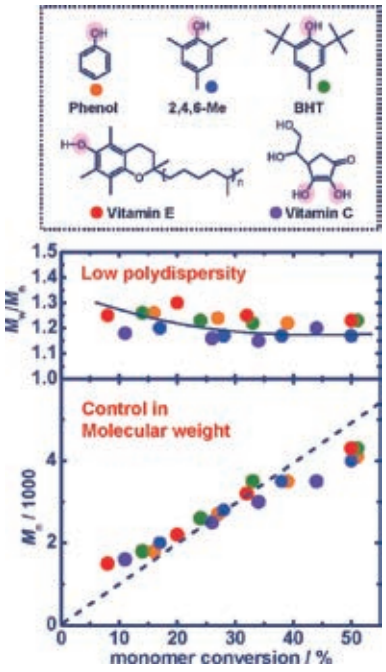


Figure 2. Plots of molecular weight (M_n) and molecular weight distribution (M_w/M_n) vs monomer conversion for the polymerizations of styrene with alcohols (catalysts).

Development of High-Performance Battery System for Next-Generation Vehicles by NEDO, 1 July 2007–20 March 2008.

Tsujii Y, R&D of High-Efficient Organic Thin-Film Solar Cell with Supra-Hierarchical Nano-Structure, R&D for Next Generation PV System Technologies by NEDO, 1 September 2006–20 March 2010.

Ohno K, Science of Semi-Soft Colloidal Crystals, Grant-in-Aid for Young Scientists (A), 1 April 2005–31 March 2008.

Goto A, Non-Transition-Metal Catalyzed and Photo-Induced LRPs, Grant-in-Aid for Young Scientists (B), 1 April 2007–31 March 2009.

Goto A, Development of Green LRP with Low Cost, Industrial Technology Research Grant Program by NEDO, 10 September 2007–31 August 2011.

Goto A, Fundamentals and Applications of Non-Transition-Metal Catalyzed LRP, Mitsubishi Chemical Corporation Fund, 1 November 2007–31 August 2008.

Goto A, Development of New LRP, JST Promotion of Technology Research Partnership, 10 August 2008–31 July 2009.

Award

Goto A, Young Scientist Presentation Award, 54th Annual Kobe Polymer Research Symposium, 18 July 2008.

Division of Materials Chemistry
- Polymer Controlled Synthesis -

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

Prof
YAMAGO, Shigeru
(D Sc)

Assoc Prof
TSUJI, Masaki
(D Eng)

Assist Prof
TOSAKA, Masatoshi
(D Eng)

Assist Prof
NAKAMURA, Yasuyuki
(D Sc)

PD
KOTAL, Atanu
(Ph D)

Students

KAYAHARA, Eiichi (D1)
UKAI, Yu (M2)
YAMAGUCHI, Katsuya (M2)
UEKI, Kazuya (M1)
YAMADA, Hiroto (M1)
YANG, Junyue (M1)
WATANABE, Yoshiki (M1)
UEDA, Tokiko (UG)
OKUMURA, Yusuke (UG)
KONISHI, Shota (UG)
FUJITA, Takehiro (UG)

Visitors

Prof LEE, Jae-Suk	Gwangju Institute of Science and Technology, Korea, 31 January 2008
Prof HANDA, Sandeep	University of Leicester, UK, 11 March 2008
Prof CRUDDEN, Cathleen	Queen's University, Canada, 20 May 2008
Prof NOZAKI, Kyoko	The University of Tokyo, Japan, 16–17 September 2008
Prof HVILSTED, Søren	Technical University of Denmark, Denmark, 10 November 2008
Prof KIM, Byeang Hyean	Pohang University of Science and Technology, Korea, 10 November 2008
Prof LOH, Tech Peng	Nanyang Technological University, Singapore, 11 December 2008

Scope of Research

Our research program focuses on development of new synthetic methods, which enable precise control of polymers in terms of their size and structure. Our attention is especially directed to control of reactive carbon species, such as carbon centered radicals and carbocations, with the aid of synthetic organic chemistry, element chemistry, computational chemistry, and so on. We also study various polymer condensed states by both static and dynamic methods to understand the relation of physical properties and structures.

Research Activities (Year 2008)

Publications

Kayahara E, Yamago S, Kwak Y, Goto A, Fukuda T: Optimization of Organotellurium Transfer Agents for Highly Controlled Living Radical Polymerization, *Macromolecules*, **41**, 527-529 (2008).

Yamada T, Mishima E, Ueki K, Yamago S: Phenyltellanyl Triflate (PhTeOTf) as a Powerful Tellurophilic Activator in the Friedel-Crafts Reaction, *Chem. Lett.*, 650-651 (2008).

Yamago S, Matsumoto A: Arylthiols as Highly Chemoselective and Environmentally Benign Radical Reducing Agents, *J. Org. Chem.*, **73**, 7300-7304 (2008).

Yamago S, Yamada T, Togai M, Ukai Y, Kayahara E, Pan N: Synthesis of Structurally Well-Defined Telechelic Polymers by Organostibine-Mediated Living Radical Polymerization. *In Situ* Generation of Functionalized Transfer Agents and Selective ω-End Group Transformations, *Chem. Eur. J.* (in press).

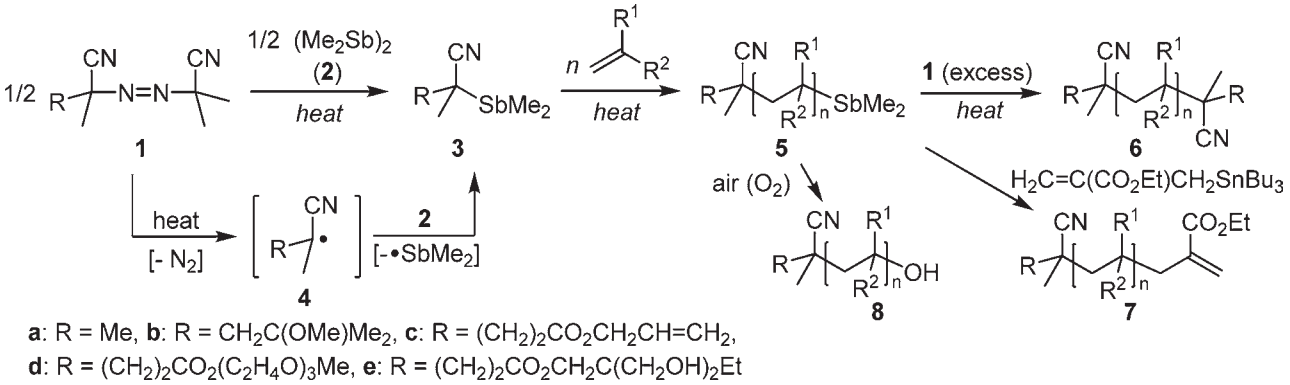
Presentations

"A New Thiobismuthine Cocatalyst in Organobismuthine-Mediated Living Radical Polymerization", Yamago S, Kayahara E, American Chemical Society National Meeting, 5th Controlled/Living Radical Polymerization Symposium, Philadelphia, USA, 17–21 August 2008 (invited).

"Reinforcing Effect of Strain-Induced Crystallization in Natural Rubber", Tosaka M, The 144th Symposium on Rubber Technology, Tokyo, Japan, 20 August 2008 (invited).

Synthesis of Structurally Well-Defined Telechelic Polymers by Organobismuthine-Mediated Living Radical Polymerization

There has been growing interest in new synthetic methods for the preparation of well-defined polymers with controlled chain-end functional groups. These end-functional polymers, as exemplified by telechelic polymers, serve as precursors not only for block and graft copolymers, but also for cyclic, branched, and cross-linked polymers. We have recently reported organostibine compounds mediate living radical polymerization with varieties of vinyl monomers. While introduction of functionality into the chain transfer agents would enhance the abilities for the synthesis of telechelic polymers, strong basic conditions required for preparation of the transfer agents have limited this possibility. We report here a new synthetic route to organostibine chain transfer agents from diazo-initiators and distibines. As the synthesis proceeds under neutral conditions, a variety of polar functional groups can be introduced into the chain transfer agent and, thus, the α-polymer ends. Subsequent transformation of the organostibine ω-polymer ends provids structurally well-defined telechelic polymers.



a: R = Me, **b**: R = $CH_2C(OMe)Me_2$, **c**: R = $(CH_2)_2CO_2CH_2CH{=}CH_2$,
d: R = $(CH_2)_2CO_2(C_2H_4O)_3Me$, **e**: R = $(CH_2)_2CO_2CH_2C(CH_2OH)_2Et$

Figure 1. Synthesis of telechelic polymers by organostibine-mediated living radical polymerization.

"Synthesis of Structurally Well-Defined Telechelic Polymers by Organostibine-Mediated Living Radical Polymerization. *In Situ* Generation of Functionalized Chain Transfer Agents and Selective End Group Transformations", Yamago S, 18th International Symposium on Fine Chemistry and Functional Polymers & IUPAC 4th International Symposium on Novel Materials and Synthesis, Zhenjiang, China, 15–18 October 2008 (invited).

"Synthesis of Structurally Well-Defined Telechelic Polymers by Organostibine-Mediated Living Radical Polymerization", Yamago S, The 2nd Japan-Korea Joint Seminar 2008 and International Symposium. Synthetic Application of Advanced Functional Materials, Tokyo, Japan, 6–7 November 2008 (invited).

"Taming Radical Species. Development of Living Radical Polymerization Mediated by Heavier Organoheteroatom Compounds", Yamago S, The 4th RIKEN Symposium on Frontier of Organometallic Chemistry, Wako, Japan, 14 November 2008 (invited).

"Organotellurium Mediated Living Radical Polymerization Initiated by Direct C-Te Bond Photolysis", Yamago S, International Symposium on Advanced Green Catalysis and Materials, Taipei, Taiwan, 18–19 November 2008 (invited).

"Synthesis of Structurally Well-Defined Telechelic Polymers by Organostibine-Mediated Living Radical Polymerization", Yamago S, Post-ISOR Symposium, Taipei, Taiwan, 24 November 2008 (invited).

Grants

Yamago S, Precise Control of Radical Reactions Using Synergetic Effects of "Heavy" Heteroatom Compounds, Grant-in Aid on Priority Areas, 1 October 2006–31 March 2010.

Yamago S, Torey Science Foundation, Torey Science and Technology Grant, 1 April 2008–31 March 2010.

Yamago S, Nagase Science and Technology Foundation Grant, 1 April 2008–31 March 2009.

Tsuji M, Structure Analysis of Poly(dioxanone) Nanofibers Prepared by Electro-Spinning Method, Grant-in Aid for Scientific Research, (C), 1 April 2007–31 March 2009.

Tosaka M, Near-Field Optical Effects of Self-Assembled Nanoparticle Chains on Oriented Polymer Layers, The Ogasawara Foundation for the Promotion of Science & Engineering Grant, 1 April 2007–31 March 2008.

Tosaka M, Formation of Nanoparticle Arrays Using Alignment of Polymer Molecules, Grant-in Aid for Scientific Research, (C), 1 April 2008–31 March 2011.

Division of Materials Chemistry
- Inorganic Photonics Materials -

http://noncry.kuicr.kyoto-u.ac.jp/English/Welcome.html

Prof
YOKO, Toshinobu
(D Eng)

Assoc Prof
TAKAHASHI, Masahide
(D Sc)

Assist Prof
TOKUDA, Yomei
(D Eng)

PD (JSPS)
IHARA, Rie
(D Eng)

Guest Res Assoc
FIGUS, Cristiana

Researcher

FUKUDA, Masaaki

Students

OKA, Takanori (M2)
OKU, Satoshi (M2)
MIYAGAWA, Yuya (M2)
OHTA, Masayuki (M1)
INOUE, Masafumi (M1)
SHINAGAWA, Masashi (M1)
MORITA, Masanori (UG)
NISHIOKA, Satoshi (UG)

Visitors

Prof INNOCENZI, Plinio — University of Sassari, Italy, 15 July 2008–1 August 2008
Prof QIU, Jianrong — Zhejiang University, China, 12 June 2008

Scope of Research

In this laboratory, amorphous and polycrystalline inorganic materials and organic-inorganic hybrid materials with various optical functions such as photorefractivity, optical nonlinearity, phptolumionescence and photocatalysis are the target materials, which are synthesized by sol-gel, melt-quenching and sintering methods and so on. Aiming at highly functional materials the structure-property relationship is investigated by X-ray diffraction techniques, high-resoluction NMR, thermal analysis, various laser spectroscopies and quantum chemical calculations.

Research Activities (Year 2008)

Publications

Takahashi M, Uemura K, Maeda T, Yao J, Tokuda Y, Yoko T, Costacurta S, Malfatti L, Innocenzi P: Bottom-up and Top-down Approach for Periodic Microstructures on Thin Oxide Films by Controlled Photo-activated Chemical Processes, *J. Sol-Gel Sci. Tech.*, **48**, 182-186 (2008). (invited paper)

Falcaro P, Costacurta S, Malfatti L, Takahashi M, Kidchob T, Casula M F, Piccinini M, Marcelli A, Marmiroli B, Amenitsch H, Schiavuta P, Innocenzi P: Fabrication of Mesoporous Functionalized Arrays by Integrating Deep X-ray Lithography with Dip-pen Writing, *Adv. Mat.,* **20(10)**, 1864-1869 (2008). (Featured on "Advances in Advance")

Presentations

Takahashi M, "Patterning Technology for Sol-Gel Films", ISGS Sol-Gel School "Sol-Gel in Small Dimensions", Italy, 24–27 August 2008 (invited).

Takahashi M, "Self-oraganized Fabrication of Microstructures on Sol-Gel Derived Films", Deajion, Korea, 3–6 December 2008 (invited).

Tanaka Y, Tokuda Y, Takahashi M, Yoko T, "Preparation of the Durable Organic-inorganic Hybrid Silicophosphate Glasses", Annual Meeting of The Ceramic Society of Japan, 20–22 March 2008.

Grants

Yoko T, Grants-in-Aid for the Scientific Research from Japan Society for the Promotion of Science, No. 20613007.

Development of Alternating Copolymers of Organically-Modified Oxides Prepared by Nonsolvent Condensation

Organic-inorganic hybrid materials are potential candidates for use in the fabrication of electronic and photonic devices with high functionality because these materials can be processed easily and have a high solubility of functional molecules. Recently, an organic-inorganic silicophosphate hybrid has been obtained under a nonsolvent, catalyst-free, low-temperature, one-pot condition by using orthophosphoric acid and organically modified chlorosilane. The following acid-base reaction (metathesis) took place: Si–Cl + P–OH → Si–O–P + HCl↑. The starting materials were mixed and heat-treated at low temperature. The resultant viscous liquid was cooled down to an ambient temperature, producing a transparent bulk hybrid material that provided an alternating polymerized silicophosphate structure with a high homogeneity at the atomic level. The crack-free bulk hybrid material was easily obtained because of the absence of solvent evaporation. However, this reaction produces HCl gas, which is both toxic and caustic. Additionally, the residual HCl gas in the hybrid material may act as a catalyst for the hydrolysis of Si–O–P bonding, resulting in low durability. Thus, the silicophosphate hybrid prepared by the acid-base reaction is not durable.

In this study, we will develop another class of low-melting silicophosphate hybrid formation reaction that is based on nonsolvent alcohol condensation without HCl production: Si–OEt + P–OH → Si–O–P + EtOH↑. The chemical durability of the hybrid was higher than that of the hybrid prepared by using the acid-base reaction. We also investigated the transition state structure of the hydrolysis. It was found that the residual acid assisted the hydrolysis of the hybrids. On the basis of this result we concluded that the durability improvement was performed because of no residual acid in the hybrids prepared by alcohol condensation.

Self-Organized Nanocrystalline Organosilicates in Organic-Inorganic Hybrid Films

Organic-inorganic hybrid films containing organosilica nanocrystals have been obtained by an aqueous process from an organically modified mono-functional alkoxide. Kinetically controlled self-organization was used to design the hybrid nanocomposite films; nanocrystals of around 100 nm in diameter and 4 nm in thickness formed in transparent hybrid films. The layered nanocrystals was found to be oriented within the films which exhibited an optical anisotropy ($\Delta n > 10^{-3}$). Therefore, the hybrid nanocomposite material is thought to be suitable for micro/nanofabrication by soft lithography. In fact the hybrid nanocomposite films with different patterned microstructures have been obtained.

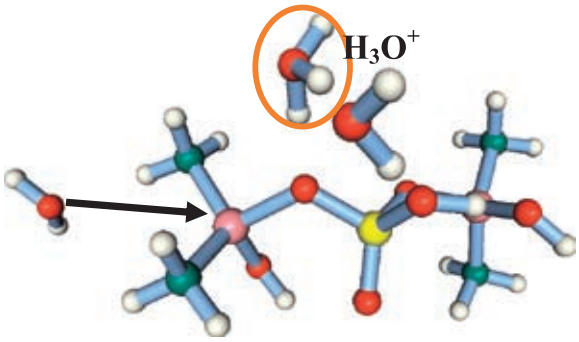


Figure 1. A transition state structure of the hydrolysis of the silicophophate hybrid. The geometry optimization was performed at B3LYP/6-31G* level. It has been found that the oxonium ion promotes the hydrolysis of this model cluster.

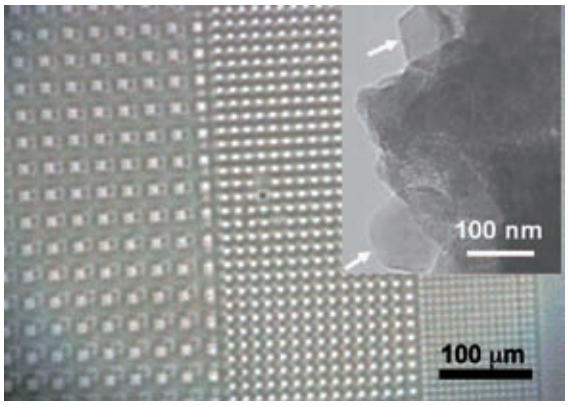


Figure 2. Optical microscope image of the patterned hybrid film containing the layered organosilica nanocrystals micro-fabricated by a soft-lithography. Inset shows TEM image of the corresponding patterned film, in which nanocrystallites are indicated by arrows.

Tokuda Y, CASIO Science Promotion Foundation, December 2007–November 2008.

Tokuda Y, Murata Science Foundation, July 2008–March 2009.

Award

Takahashi M, Award for Promising Young Researchers, The Ceramics Society of Japan, Kansai Branch, 24 July 2008.

Division of Materials Chemistry
- Nanospintronics -

http://ssc1.kuicr.kyoto-u.ac.jp/english/index_e.html

Prof
ONO, Teruo
(D Sc)

Assoc Prof
KOBAYASHI, Kensuke
(D Sc)

Assist Prof
KASAI, Shinya
(D Sc)

Program-Specific Assist Prof
CHIBA, Daichi
(D Eng)

Techn
KUSUDA, Toshiyuki

Program-Specific Res
SEKIGUCHI, Koji
(D Sc)

Students

TANIGAWA, Hironobu (D3)
HASHISAKA, Masayuki (D3)
DELMO, Michael Picazo (D2)
TAMADA, Yoshinori (D2)
YAMAUCHI, Yoshiaki (D2)
KONDOU, Kouta (D1)
NAKAMURA, Shuji (D1)
YAMADA, Keisuke (D1)
KOYAMA, Tomohiro (M2)
NAKANO, Kunihiro (M2)
TANABE, Kenji (M1)
CHIDA, Kensaku (M1)
YAMADA, Gen (M1)
BARTKOWIAK, Maciej (M1)

Scope of Research

The conventional electronics utilizes only the "charge" of electrons, while the traditional magnetic devices use only "spin" degree of freedom of electrons. Aiming at the complete control of both charge and spin in single solid-state devices, 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.

Research Activities (Year 2008)

Publication

Tanigawa H, Koyama T, Bartkowiak M, Kasai S, Kobayashi K, Nakatani Y, Ono T: Dynamical Pinning of a Domain Wall in a Magnetic Nanowire Induced by Walker Breakdown, *Physical Review Letters*, **101**, 207-203 (2008).

Presentations

Current-induced Spin Dynamics in Nanomagnet, Ono T, International Workshop on "SPIN CURRENT 2008", 18–19 February 2008, Sendai, Japan.

Detection of Shot Noise in Coupled Mesoscopic Systems, Kobayashi K, International Workshop "Interaction and Interference in Nanoscopic Transport",18–23 February 2008, Dresden, Germany.

Coherence and Correlation of Electrons in Quantum Hybrid Systems, Kobayashi K, Moriond 2008, "Quantum Transport and Nanophysics", 8–15 March 2008, La Thuile, Italy.

Current-induced Resonant Motion of the Magnetic Vortex Core in a Ferromagnetic Circular Disk, Kasai S, International Magnetic Conference "Intermag Europe 2008", 4–8 May 2008, Madrid, Spain.

Current-induced Vortex Core Motion in Magnetic Disk, Ono T, Moscow International Symposium on Magnetism, 20–25 June 2008, Moscow, Russia.

Current-induced Magnetization Dynamics in Nanomagnet, Ono T, The 5th Asia Forum on Magnetics, 16–19 October 2008, Beijing, China.

Grants

Ono T, Invention of Anomalous Quantum Materials, Grant-in-Aid for Scientific Research in Priority Areas, 1 April 2004–31 March 2010.

Ono T, Magneto-transport Engineering by Spin-polarized Current, The Asahi Glass Foundation, 1 April 2005–31 March 2008.

Ono T, Current-induced Spin Dynamics and its Application to Spintronic Devices, Grant-in-Aid for Young Scientists (S), 1 October 2007–31 March 2012.

Kobayashi K, Generation and Detection of Quantum

Real-time Imaging of the Current-driven Vortex-core Motion

Manipulating magnetization by spin currents is attracting scientific interest both due to the intricate physics involved in the interaction between the flowing spins and the localized spins that constitute magnetization and the technological potential to control future nanoscale spintronics devices. Since the efficiency of this spin torque effect is proportional to the spin-polarization of the current flowing in the ferromagnetic material an experimental quantification of the spin-polarization is of paramount importance. So far, the indirect methods used, i.e. transport measurements, such as tunneling spectroscopy, Andreev reflection, and giant magnetoresistance measurements have not shown conclusive results. Recently by using the at beamline 6.1.2 at the Advanced Light Source (ALS) in Berkeley we succeeded in a direct determination of the spin-polarization of the currents from quantitative high resolution X-ray imaging of the current-induced circular motion of a vortex core in a ferromagnetic disk (Figure 1). We are able to watch the motion of the core position with better than 25 nm spatial resolution with a 70 ps time resolution over a period of several nano-seconds. The spin-polarization of the current is determined to be 0.67 for Permalloy ($Fe_{19}Ni_{81}$), which is in excellent agreement with an analytical model in the framework of the spin transfer torque.

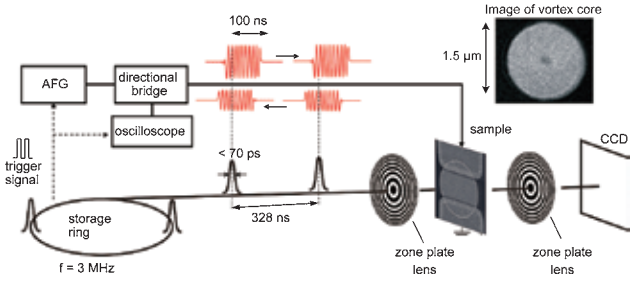


Figure 1. Schematic illustration of the experimental setup for imaging the spin dynamics by time- and space-resolved magnetic soft X-ray microscopy of the vortex core motion in a Permalloy disk (diameter: 1.5 μm; thickness: 40 nm).

New Scheme for the Quantum Noise Detection: Mesoscopic Bolometry

Coupled mesoscopic systems offer exciting opportunities to generate and control quantum correlations between electrons, which constitute an important step towards the integration of quantum optics and electronics. To explorer the interaction mediated by photons is one of the most imperative issues because well-prepared photons can link separate systems quantum-mechanically and, otherwise, they undesirably disturb the quantum state. We present a new scheme to detect the photon exchange between the systems by means of the precise noise thermometry; in the coupled quantum point contacts (QPC) we prove that the temperature of one QPC, where the single quantized conducting channel works as a photon detector, is in perfect proportion to that of the other QPC which is driven to non-equilibrium to emit photons (Figure 2). The present on-chip bolometry opens up a new way for the detection of the quantum correlation created by photons and for the attractive ultra-precise measurements such as the bolometric photon counting and the advanced metrology.

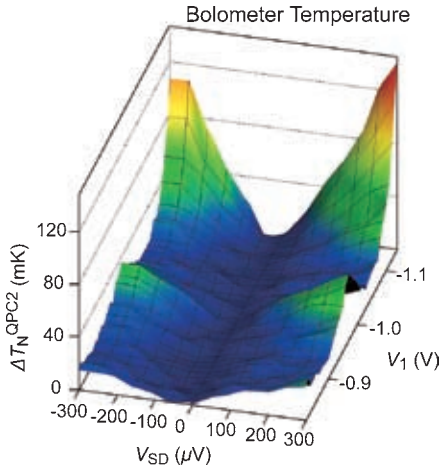


Figure 2. The experimental result of the bolometric detection of the quantum noise is shown in 3D image plot.

Correlation in Semiconductor Nanostructures, Grant-in-Aid for Young Scientists (S), 1 October 2007–31 March 2012.

Awards

Ono T, FFIT Prize, Development of the Magnetization Control Technology by Electric Currents, Funai Foundation for Information Technology, 19 April 2008.

Ono T, The 10th Sir Martin Wood Prize, Magnetization Control in Nano-Magnets by Electric Currents, Millennium Science Forum, 12 November 2008.

Ono T, Japan IBM Prize, Research on the Magnetization Control by Spin-polarized Currents, 26 November 2008.

Kasai S, Young Author Presentation Awards, Time-resolved Measurement of the Current-induced Vortex Core Dynamics in a Ferromagnetic Circular Disk, The Japan Society of Applied Physics, 29 March 2008.

Hashisaka M, IUPAP Young Author Best Paper Awards, Bolometric Shot Noise Detection in Coupled Quantum Point Contacts, The 29th International Conference on the Physics of Semiconductors, 1 August 2008.

Division of Biochemistry
- Biofunctional Design-Chemistry -

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

Prof
FUTAKI, Shiroh
(D Pharm Sc)

Assist Prof
IMANISHI, Miki
(D Pharm Sc)

Assist Prof
NAKASE, Ikuhiko
(D Pharm Sc)

PD
TANAKA, Gen
(D Eng)

Students

MORISAKI, Tatsuya (D2)
NAKAMURA, Atsushi (D1)
TAKAYAMA, Kentaro (D1)
AZUMA, Yusuke (M2)
HIROSE, Hisaaki (M2)
KOBAYASHI, Sachiko (M2)
NAKAMURA, Yasunori (M2)
NOSHIRO, Daisuke (M2)
IMAMURA, Chika (M1)
KATAYAMA, Sayaka (M1)
KONISHI, Yusuke (M1)
TATSUTANI, Kazuya (M1)
TSUDA, Nami (M1)
YU, Hao-Hsin (RS)
HIROSE, Yuka (UG)
KOGA, Makito (UG)
MIYAMAE, Hiroki (UG)
NOGUCHI, Haruka (UG)

Visitors

Prof PROCHIANTZ, Alain Louis — École Normale Supérieure, France, 24 September 2008
Prof GRASLUND, Astrid — Stockholm University, Sweden, 14 October 2008

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-responsible artificial peptides and proteins.

Research Activities (Year 2008)

Presentations

"Cellular Dynamics of Cell Penetrating Peptides", Futaki S, 2nd International Symposium "Cellular Delivery of Therapeutic Macromolecules 2008", Cardiff, UK, 24 June 2008.

"Effective Macropinocytosis Induction and Membrane Penetration by FHV Peptide", Nakase I, Hirose H, Takeuchi T, Futaki S, Cell-Penetrating Peptides (CPP) Satellite Symposium of 30th European Peptide Symposium, Helsinki, Finland, 31 August 2008.

"Novel Intracellular Delivery System using pH-Dependent Fusiogenic Peptide", Nakase I, Kobayashi S, Kawabata N, Futaki S, 30th European Peptide Symposium, Helsinki, Finland, 5 September 2008.

"Arginine-Rich Peptides as a Vector of Intracellular Delivery" Futaki S, 3rd International Workshop on Approaches to Single-Cell Analysis, Zurich, Switzerland, 12 September 2008.

"Internalization of Arginine-Rich Peptides into Cells", Futaki S, The 6th China-Japan-Korea Foresight Joint Symposium on Gene Delivery and International Symposium on Biomaterials, Sanya, China, 26 November 2008.

Grants

Futaki S, Chemical Biology in Translocation of Membrane Permeable Peptides into Cells, Grant-in-Aid for Scientific Research (A), 1 April 2007–31 March 2010.

Futaki S, Developing Methodologies of Efficient Intracellular Delivery for Cell Imaging and High-Throughput Analysis, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2007–31 March 2009.

Imanishi M, Screening and Evaluation of Novel Clock-

Efficient Cellular Uptake of Flock House Virus Derived Arginine-Rich Peptide

Arginine-rich cell penetrating peptides (CPPs), including HIV-1 Tat (48-60) and oligoarginine peptides, have been applied for intracellular delivery of various molecules (e.g., bioactive proteins, peptides, nucleic acids). Macropinocytosis has been shown to be one of the major pathways in the CPP internalization, and we have already reported that interaction of CPPs with membrane-associated proteoglycans leads actin organization and the eventual induction of macropinocytosis.

From the study on cellular uptake efficiency of various DNA/RNA binding peptides rich in arginines, we have found that a peptide derived from flock house virus coat protein [FHV coat (35-49): RRRRNRTRRNRRRVR] internalized ~20 times more efficiently than Tat peptide into Chinese hamster ovary (CHO-K1) cells. The FHV peptide (1 μM) was able to induce similar extent of macropinocytosis to that of the Tat peptide (10 μM), and extent of cell surface adsorption of the FHV peptide was also considerably higher than that of the Tat peptide. Additionally, when the cells were treated with Alexa-labeled FHV peptide (10 μM) for 10 min, the peptide could translocate into cytosol and nucleus efficiently. On the other hand, only endosome-like signals were observed in the case of the Tat peptide by a confocal microscopy. These results suggest that effective macropinocytosis induction by the FHV peptide would lead its efficient internalization.

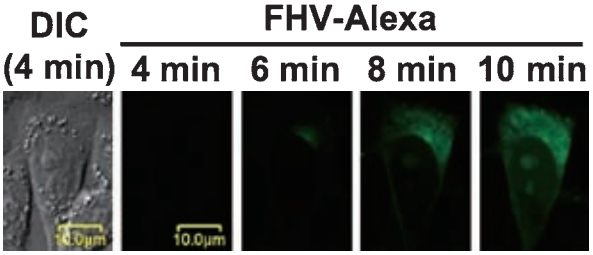


Figure 1. Confocal microscopic observation of CHO-K1 cells treated with Alexa-labeled FHV peptide (10 μM) at 37 °C. Times show incubation periods of the peptide on cells.

Rapid Transcriptional Activity *in Cellulo* and Slow DNA Binding *in Vitro* by Artificial Multi-Zinc Finger Protein

Artificial transcription factors targeting any desired genes are very attractive, but require specific DNA binding domains in order to address a single site for each gene promoter. By connecting various zinc fingers recognizing the corresponding 3- to 4-bp DNA, DNA binding domains for the desired and long sequences can be created. Though such a long sequence recognition is a marvelous property, we have found as the number of finger motifs increases, the equilibrium time with the target sequence is significantly longer as detected by *in vitro* EMSA experiments. In this study, we created 3- and 9-finger type artificial transcription factors, and compared the kinetics of the transcriptional activation *in vivo* as to whether or not a significant delay in the activation is observed for the 9-finger type. By using a ligand-inducing system, we demonstrated for the first time that finger multimerization does not affect the kinetics of the transcriptional activity; the 9-finger type artificial transcription factor activated the reporter gene as quickly as the 3-figner type. Our results suggest that the drawback of finger multimerization, i.e., the equilibrium time is prolonged depending on the number of finger motifs, can be surmounted in terms of its use for transcription factors *in vivo*. There is much interest in creating therapeutic molecules, and these findings suggest the significant potential of multi-zinc finger proteins as a tool for an artificial gene regulator.

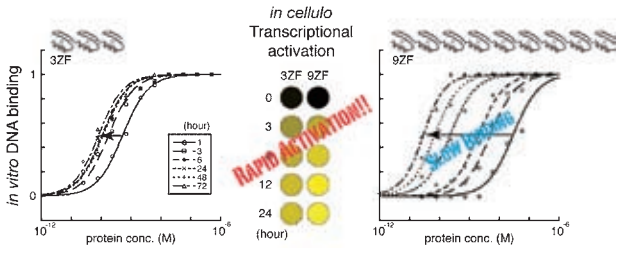


Figure 2. Rapid Transcriptional Activation by an Artificial Multi-Zinc Finger Protein.

Related Proteins Using Zinc-Finger Technology, PRESTO Program, Japan Science and Technology Agency, 1 October 2005–31 March 2009.

Nakase I, Development of New Cell-Targeting Peptides Having Functional Activities for Recognition of Various Proteoglycans on Cell Membrane, Grant-in-Aid for Young Scientist (B), 1 April 2007–31 March 2009.

Award

Imanishi, M, The Best Poster Prize, Chemistry in the New World of Bioengineering and Synthetic Biology (Royal Society of Chemistry), Oxford, UK, 24 September 2008.

Division of Biochemistry
- Chemistry of Molecular Biocatalysts -

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

Prof
HIRATAKE, Jun
(D Agr)

Assist Prof
MIZUTANI, Masaharu
(D Agr)

Assist Prof
SHIMIZU, Bun-ichi
(D Agr)

Students

IKEUCHI, Hideyuki (M2)
KAWABE, Ayami (M2)
NAITO, Yoshiyuki (M2)
NAKAJIMA, Mado (M2)
MATSUMOTO, Seitaro (M2)
ASAI, Tomoki (M1)
YANG, Qing-Hua (RS)

Scope of Research

Our research covers the comprehensive understanding of the physiological roles of biocatalysts (enzymes) as well as the reaction mechanism, the structure and properties of each enzyme. 1) Development of intermediate analogue inhibitors of acyl-activating enzyme superfamily that plays pivotal roles in plant hormone homeostasis and secondary metabolite biosynthesis of plants. 2) Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ- glultamylcysteiene synthetase and γ-glutamyl transpeptidase, the key enzymes in glutathione biosynthesis and its metabolism, respectively. 3) Studies on structural basis for bioluminescence change of firefly luciferase. 4) Studies on the activation/inactivation process of plant hormones. 5) Molecular mechanism of regulation of coumarin biosynthesis in plants.

Research Activities (Year 2008)

Publications

Wada K, Hiratake J, Irie M, Okada T, Yamada C, Kumagai H, Suzuki H, Fukuyama K: Crystal Structures of *Escherichia coli* γ-Glutamyltranspeptidase in Complex with Azaserine and Acivicin: Novel Mechanistic Implication for Inhibition by Glutamine Antagonists, *J. Mol. Biol*., **380**, 361-372 (2008).

Saino H, Mizutani M, Hiratake J, Sakata K: Biochemical Characterization of β-Primeverosidase–Expression with a Baculovirus Insect Cell System and Affinity Purification with a Primeverosylamidine as a Ligand–**,** *Biosci. Biotechnol. Biochem*., **72**, 376-383 (2008).

Kai K, Mizutani M, Kawamura N, Yamamoto R, Tamai M, Yamaguchi H, Sakata K, Shimizu, B: Scopoletin is Biosynthesized via *ortho*-Hydroxylation of Feruloyl-CoA by an 2-Oxoglutarate Dependent Dioxygenase in *Arabidopsis thaliana*, *Plant J*., **55**, 989-999 (2008).

Seki H, Ohyama K, Sawai S, Mizutani M, Ohnishi T, Sudo H, Akashi T, Aoki T, Saito K, Muranaka T: Licorice β-Amyrin 11-Oxidase, a Cytochrome P450 with a Key Role in the Biosynthesis of the Triterpene Sweetener Glycyrrhizin, *Proc Natl Acad Sci USA*., **105**, 14204- 14209 (2008).

Presentations

Rational Design of Specific Inhibitors of γ-Glutamyl Transpeptidase (GGT) and γ-Glutamylcysteine Synthetase for Modulating Cellular Glutathione Redox Status, Hiratake J, 2nd World Conference on Magic Bullets (Ehrlich II), Nuernberg, Germany, 4 October 2008.

Biochemical Characterization of Cytochrome P450 Monooxygenases in Plant Steroid Metabolism, Mizutani M, 7th Japan-US Seminar, Biosynthesis of Natural Products, "Enzymology, Structural Biology, and Drug Discovery", San Diego, USA, 24 June 2008.

New Functions of P450s in Brassinosteroid Biosynthesis and Catabolism, Mizutani M, 9th International Symposium on Cytochrome P450 Biodiversity and Biotechnology, Nice, France, 10 June 2008.

Molecular Design and Synthesis of γ-Glutamylcysteine Synthetase Inhibitors

γ-Glutamylcysteine synthetase (GCS) catalyzes the ATP-dependent coupling of L-Glu and L-Cys to make γ-Glu-Cys, the first and the rate-limiting step in glutathione biosynthesis. Therefore GCS is an extremely important enzyme that controls the cellular redox status and detoxification potential through affecting the glutathione level and confers the cells with resistance against toxic xenobiotics such as reactive oxygen species and anticancer drugs. We designed and synthesized the sulfoximine-based transition-state analogue inhibitors **1a** and **b** with an emphasis on the recognition of the side chain of Cys by the enzyme [Figure 1. (a)]. The X-ray crystallographic studies on *E. coli* GCS indicated that the side chain of Cys was recognized by Arg132 [Figure 1. (b)]. The inhibitor **1b** with a cyano group at the side chain of Cys moiety was ca. 5 times more potent than the inhibitor **1a** with a methyl group, suggesting that the cyano group mimicked the SH of Cys to interact with the guanidino group of Arg132. The cyano sulfoximine **1b** was more than 6000 times as potent as buthionine sulfoximine (BSO), a most frequently used GCS inhibitor, thus serving as a new lead for effective drug for controlling the cellular glutathione biosynthesis.

Cytochrome P450s in Brassinosteroid Biosynthesis

Brassinosteroids (BRs) are plant steroid hormones that are essential for normal growth and development in plants. Cytochrome P450 monooxygenases (P450s) play crucial roles in BR biosynthesis, in which many oxygenations at steroidal skeleton and side-chain structure occur. Recent molecular genetic studies for BR-deficient mutants of Arabidopsis, rice, tomato, and garden pea have identified several P450 genes (*CYP85A, 90A, 90B, 90C, 90D*, and *724B*) so far. However, the catalytic functions of them remained ambiguous due to lack of biochemical study. Recently, we succeeded in functional expression of these P450s in a baculovirus-insect cell system as well as in a bacterial expression system, and their catalytic activities were determined in an *in vitro* assay. We found that *CYP90B* and CYP724B are redundant C-22 hydroxylases and also that CYP90C and CYP90D are redundant C-23 hydroxylases. CYP90A was found to catalyze C-3 oxidation and isomerization of 22-hydroxycampesterol and 22,23-dihydroxycampesterol to produce their corresponding 4-en-3-one. In contrast, campesterol is not metabolized by CYP90A at all. Taken together, we have proposed the campestanol-independent pathway of BR biosynthesis, which predominantly converts campesterol to 22-hydroxycampesterol and (22*S*,24*R*)-22-hydroxyergost-4-en-3-one to form bioactive BRs, without going through campestanol.

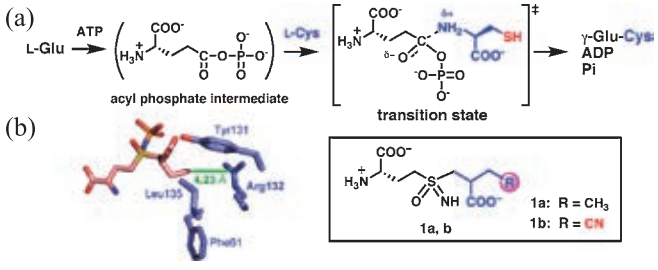


Figure 1. (a) The reaction mechanism of GCS and the sulfoximine-based transition-state analogue inhibitors **1a** and **1b**. (b) The X-ray structure showing the interaction with the side chain of Cys and Arg132.

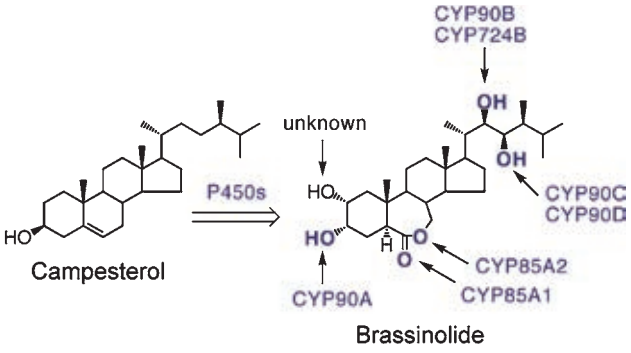


Figure 2. Cytochrome P450s in Brassinosteroid Biosynthesis CYP90A, C3-oxidase; CYP90B and CYP724B, C22-hydroxylase; CYP90C and CYP90D, C23-hydroxylase; CYP85A, C6-oxidase.

Grants

Hiratake J, Development of Chemicals to Control Glutathione Metabolism and Oxidative Stress for Use in Chemical Biology, Grant-in-Aid for Scientific Research (B) (2), 1 April 2007–31 March 2010.

Mizutani M, Construction of Plant Oxygenase Library and Its Functional Characterization, Grant-in-Aid for Scientific Research (C) (2), 1 April 2006–31 March 2008.

Division of Biochemistry
- Molecular Biology -

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

Assoc Prof
SUGISAKI, Hiroyuki
(D Sc)

Assoc Prof
AOYAMA, Takashi
(D Sc)

Assist Prof
TSUGE, Tomohiko
(D Sc)

Techn
YASUDA, Keiko

PD
TANIGUCHI, Masatoshi
(D Sc)

Guest Res Assoc
WU, Zhe

Guest Res Assoc
ZHU, Danling

Students

TANIGUCHI Y, Yukimi (D3)
NAKAMURA, Kinu (D3)
AKI, Shiori (D2)
NAKAI, Hideto (D1)
KATAOKA, Mayuko (M2)
WADA, Yukika (M1)

Visitors

Dr MENON, Suchithra	Harvard School of Public Health, USA, 7–17 January 2008
Prof QU, Li-Jia	College of Life Science, Peking University, China, 1–13 August 2008
Prof GU, Hongya	College of Life Science, Peking University, China, 1–13 August 2008
Prof SERINO, Giovanna	University of Rome La Sapienza, Italy, 4–18 November 2008
Ms IAFRATE, Silvia	National Research Council of Italy, Italy, 4–18 November 2008

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.

Research Activities (Year 2008)

Publications

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

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

Presentations

Phospholipid Signaling in Root Hair Development, Aoyama T, Kusano H, Testerink C, Vermeer JEM, Tsuge T, Shimada H, Oka A, Munnik T, The 9th International Congress on Cell Biology, 7–10 October 2008 (Seoul).

Identification and Characterization of Novel Proteins Interacting with COP9 Signalosome Subunitl, Kataoka M, Nakai H, Taniguchi M, Aki S, Dohmae N, Heyl A, Oka A, Tsuge T, Zomes-V, 11–14 November 2008 (Yokohama).

COP9 Signalosome Interacts with RNA Processing Factors in *Arabidopsis,* Aki S, Oka A, Tsuge T, Zomes-V, 11–14 November 2008 (Yokohama).

Grants

Aoyama T, Development of Light Molecular Switch for Analyzing Intracellular Information Network, Grant-in-Aid for Exploratory Research, 1 April 2007–31 March 2009.

Aoyama T, Signal Transduction from Nutrient Conditions to Root Hair Morphogenesis, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Tsuge T, Qu LJ, Molecular Mechanism Involved in Maintaining the Flatness of the Leaf Blade, Japan-China

Roles of Phospholipid Signalings in Plant Cell Morphogenesis

Phospholipids are not only major components of the eukaryotic plasma membrane but also signaling molecules leading to a wide variety of cellular responses. Because phospholipids function as site-specific signals on membranes, they likely play pivotal roles in localizing exocytosis and the fine F-actin configuration to regions of cell expansion, such as the tips of growing root hairs. Root hairs are cellular protuberances resulting from highly polarized cell growth of specific root epidermal cells. The process of root hair growth is called tip growth, because all of the growth events including cell wall deposition and plasma membrane expansion are limited to the tip. Root hairs have been intensively studied as a model system for the molecular processes involved in plant cell morphogenesis, owing to the dispensability under laboratory conditions and accessibility for experimental observation of root hairs.

Among phospholipid signaling factors involved in plant cell morphogenesis, we focused on phosphatidylinositol 4,5-bisphosphate [PtdIns(4,5)P_2] and its producing enzyme phosphatidylinositol 4-phosphate 5-kinase (PIP5K). The localization of PtdIns(4,5)P_2 to apices of growing root hairs suggests that it is involved in tip growth. However, it is unclear how the spatiotemporal pattern of PtdIns(4,5)P_2 is established at the tip and which aspect of tip growth it regulates. We found that the *Arabidopsis thaliana PIP5K3* gene encodes PIP5K, and is expressed preferentially in root hair cells. All the T-DNA insertion mutations that we examined exhibited significantly shorter root hairs than in the wild type. Reciprocally, its overexpression caused longer root hairs in addition to multiple protruding sites on a single root hair cell. A yellow fluorescence protein fusion of PIP5K3 (PIP5K3-YFP), directed by the *PIP5K3* promoter, complemented the short root hair phenotype of the mutants, and localized intensively at the plasma membrane of elongating root hair apices, at growing root hair bulges, and notably, at sites expected to form root hair bulges. PIP5K3-YFP accumulated most in apices of root hairs elongating rapidly. These results provide evidence that PIP5K3 is involved in the localization of PtdIns(4,5)P_2 to the elongating root hair apex and acts as a key regulatory component of the machinery initiating and promoting root hair tip growth.

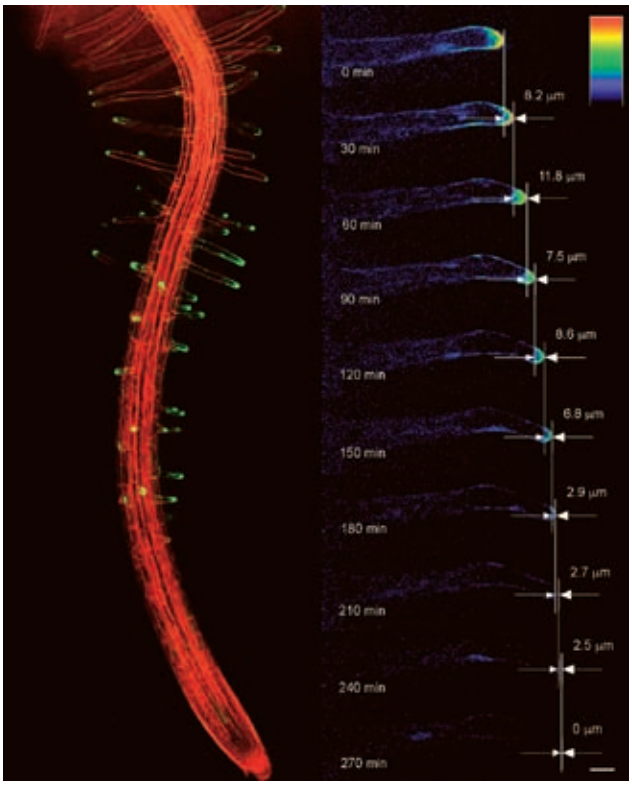


Figure 1. Localization pattern of PIP5K3-YFP in root hairs. Left: PIP5K3-YFP (green color) localized at elongating root hair apices. Right: The intensity of the PIP5K3-YFP fluorescence (index colors) is tightly correlated with the rate of root hair elongation.

Scientific Cooperation Program (JSPS), 1 April 2007–31 December 2009.

Tsuge T, Mele G, Transcriptional Regulations on Higher Plants by COP9 Signalosome, Japan-Italy Scientific Cooperation Program (JSPS), 1 April 2008–31 March 2010.

Tsuge T, Stress-response Regulator, COP9 Signalosome, is Involved in Regulation of both Human Carcinogenesis and Plant Photomorphogenesis, Research Grant (The Naito Foundation), 1 December 2006–30 September 2008.

Tsuge T, Novel Functions of COP9 Signalosome, the Key Signaling Component is Conserved in both Human Carcinogenesis and Plant Photomorphogenesis, Research Grant (Research Foundation for Opto-Science and Technology), 1 April 2007–3 March 2009.

Aki S, Functional Analyses on the Interaction of SAP130 and COP9 Signalosome, Plant Protein Analysis Research Project Graduate-Student-Grant (NAIST Science Research and Education Promotion Unit), 1 April 2008–31 March 2009.

Award

Aki S, Best Poster Award, ZOMES-V, "COP9 Signalosome Interacts with RNA Processing Factors in *Arabidopsis* ", 14 November 2008.

Division of Biochemistry
- Chemical Biology -

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

Prof
UESUGI, Motonari
(D Pharm Sc)

Assist Prof
KAWAZOE, Yoshinori
(D Med Sc)

Assist Prof
SHIMOGAWA, Hiroki
(D Sc)

Proj Res
MURATA, Asako
(D Sc)

PD (iCeMS)
SATO, Ayato
(D Sc)

PD (iCeMS)
SATO, Shinichi
(D Eng)

PD (JSPS) (iCeMS)
KAMISUKI, Shinji
(D Sc)

Res Associates (pt)

NAKASHIMA, Mitsue (iCeMS)
ORIHARA, Tsubasa (iCeMS)

Students

SHIRAKAWA, Takashi (D2)
YAMAZOE, Sayumi (D2) (iCeMS)
KHAMBU, Bilon (D1)
SUMIYA, Eriko (D1)
TSUJIKAWA, Tomoko (M2)

Visitors

Instructor JUNG, Dongju	Baylor College of Medicine, USA, 26 March–5 April 2008
Assoc Prof TSAI, Francis TF	Baylor College of Medicine, USA, 11 November 2008

Scope of Research

In human history, small organic molecules have been utilized for improving human health and for revealing secrets of life. Discovery or design of small organic molecules with unique biological activity permits small-molecule-initiated exploration of biology and further understanding of human diseases. Our laboratory has been discovering small organic molecules that modulate transcription or differentiation to use them as tools to explore biology. Such chemistry-initiated biology is recently called chemical biology, an emerging field of biology and medical sciences. Although our chemical biology is a basic one, it may "catalyze" future drug discovery.

Research Activities (Year 2008)

Presentations

Special Lecture: Organic Chemistry of Life, Uesugi M, Ewha Womans University, Korea, 7–11 January 2008.

Target Identification of Bioactive Small Molecules, Uesugi M, Medical Chemistry Symposium, Singapore, 23 January 2008.

Chemical Biology of Synthetic Small Molecules, Uesugi M, International Symposium on Hierarchy and Holism (ISHH): Bridging across Different Hierarchies in Natural Sciences, Okazaki, 23 February 2008.

Small-Molecule-Initiated Biology and Beyond in iCeMS, Uesugi M, AICT First International Conference on Convergence Technologies, Korea, 21 May 2008.

Chemical Biology of Synthetic Small Molecules, Uesugi M, SSF/JST-PRESTO Joint Symposium, Sweden, 27 May 2008.

Isolating and Identifying the Targets of Bioactive Small Molecules, Uesugi M, 10th Chinese International Peptide Symposium (CPS-2008), China, 2 July 2008.

Isolating and Identifying the Targets of Bioactive Small Molecules, Uesugi M, 22nd Naito Conference on Chemical Biology, Sapporo, 11 September 2008.

Small Molecule Activators of Transcription, Uesugi M, 2008 Riken Conference, Narita, 13 November 2008.

Grants

Uesugi M, Small-molecule Initiated Analysis of Cellular Signaling, Grant-in-Aid for Scientific Research (B), 1 April 2006–31 March 2008.

Uesugi M, Methods for Isolating Target Proteins of Small Molecules, Grant-in-Aid for Scientific Research on

Small-molecule-initiated Biology

Knowledge about bioactive small molecules is a treasure of the humankind. Small organic compounds that the human being have discovered or synthesized from natural resources have been utilized for improving human health and for revealing secrets of life. The major goal of our research programs has been to expand the treasure by discovering and analyzing novel organic compounds with unique biological activities and to use them as tools to explore biology.

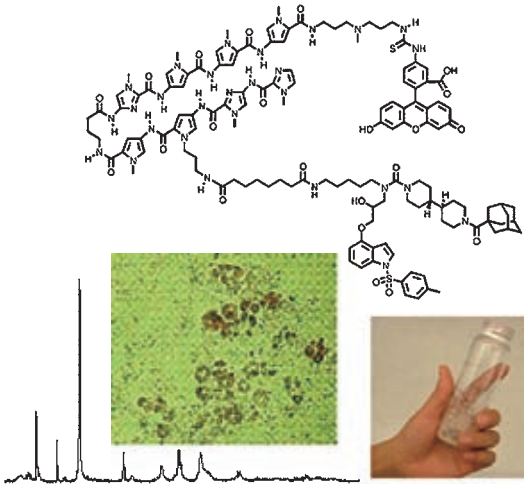
Our current research programs focus on discovering and using small organic molecules that modulate gene transcription or cell signaling. Regulation of gene transcription and cell signaling often induces drastic phenotypic changes in living organisms. Precise, external control over these endogenous processes through small organic molecules represents a challenge of chemistry to nature. The latest achievements are summarized below.

Discovery of synthetic small molecules that modulate transcription. Our group has discovered by screening chemical libraries a unique small-molecule modulator of transcription. The synthetic molecule we named "adamanolol" represents the first small molecules that modulate gene transcription by targeting transcription factor-coactivator interaction. Our group, as a collaboration with another laboratory, synthesized adamanolol and its derivatives and obtained structure-activity relationship, which enabled the design of the second-generation compound named "wrenchnolol." The wrench-shaped compound is now recognized in the field as a highly unique synthetic molecule that controls gene expression.

Wrenchnolol mimics an alpha-helical activation domain of transcription factor ESX: it may serves as a small-molecule activation module when coupled with a DNA binding molecule. Our group, as a collaboration with Prof. Dervan in Caltech, has recently succeeded in designing a completely organic, synthetic transcription factor that activates transcription. This work demonstrates that it is possible to generate a transcription factor out of organic compounds.

Discovery of small molecules that modulate cell signaling. Our group has developed an interesting method of screening chemical libararies for the discovery of bioactive molecules. In this unique method, synthetic small molecules were first profiled by their effects on phenotypic fat cell differentiation and pre-selected for more focused secondary assays. This approach enabled us to discover a number of bioactive compounds with a range of biological activities, including anti-proliferation of selective cell types and inhibition of lipogenesis. These molecules are now used for elucidation of new biological pathways in our group. For example, we recently discovered a new signaling pathway to control insulin/IGF pathways by utilizing the compound we call chromeceptin.

Our group also discovered small organic molecules that differentiate mouse embryonic stem (ES) cells into dopaminergic neurons. Our approach to discovering such molecules is rooted in the logic of asymmetric catalysts in chemistry. This work might be a good demonstration of applying the logic in chemistry to the biological field.



Priority Areas, 1 April 2006–31 March 2008.

Uesugi M, Intracellular Imaging of Small Molecules, Industrial Technology Research Grant Program by NEDO, 1 June 2006–31 May 2008.

Uesugi M, Small Molecule Transcription Factors for Biological Investigations, PRESTO, Japan Science and Technology Agency, 1 October 2005–31 March 2009.

Uesugi M, Small Molecules that Promote the Production of iPS cells, The Project for Realization of Regenerative Medicine, Japan Science and Technology Agency, 1 April 2008–31 March 2013.

Kawazoe Y, Small Molecules that Modulate Cell Differentiation, Grant-in-Aid for Young Scientists (B), 1 April 2006–31 March 2008.

Kawazoe Y, Chemical Genetic Analysis of Vacuole Formation, Grant-in-Aid for Scientific Research (C), 1 April 2008–31 March 2011.

Division of Environmental Chemistry
- Molecular Materials Chemistry -

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

Assoc Prof
KAJI, Hironori
(D Eng)

Assist Prof
HIRAI, Asako
(D Eng)

Techn
OHMINE, Kyoko

Students

SUZUKI, Shinji (D3)
YAMADA, Tomonori (D3)
FUKUSHIMA, Tatsuya (D2)
SUZUKI, Furitsu (D1)
IGARASHI, Yuki (M2)
KIUCHI, Yohei (M2)
YAMANE, Hiroaki (M2)
KOUMURA, Kentaro (M1)
SHIMAHARA, Yurie (M1)
TAKAMI, Kousuke (M1)
KIMURA, Hironobu (UG)

Scope of Research

The research activities in this subdivision cover structural studies and molecular motion analyses of highly organized polymer materials in the different states by high-resolution solid-state NMR, electron microscopy, X-ray diffractometry, and so on, in order to develop high-performance and high-functionality polymer materials such as organic electron luminiscence devices and different molecular hybrid materials. The structure formation process of bacterial cellulose is also characterized in detail and environmentally friendly cellulosic nanohybrid materials are examined to develop in different stages of the biosynthesis.

Research Activities (Year 2008)

Presentations

Structure of Materials in Organic Light-Emitting Diodes Studied by Solid State NMR, Kaji H, 235th ACS National Meeting, New Orleans, LA, 9 April 2008 (Invited).

Geometric and Electronic Structures of a Hole-Transport Material, TPD, Studied by DFT Calculations and Solid-State NMR, Kaji H, Yamada T, SPIE Symposium on Photonic Devices + Applications, "Organic Light-Emitting Materials and Devices XII", San Diego, CA, 10 August 2008 (Invited).

Organic Light-Emitting Diodes Fabricated from Alq_3 in Different Crystalline Polymorphs, Kaji H, Fukushima T, The 8th International Meeting on Information Display/ International Display Manufacturing Conference 2008/ Asia Display 2008 (IMID/IDMC/ASIA DISPLAY 2008), Gyeonggi, Korea, 15 October 2008 (Invited).

Effects of Added Electrolytes on the Phase Separation Behavior in Aqueous Suspensions of Bacterial Cellulose Microfibrils and on the Magnetic Alignment of the Chiral Nematic Phase, Hirai A, Inui O, Horii F, Yamamoto S, Tsuji M, 235th ACS National Meeting, New Orleans, LA, 7 April 2008 (Invited).

Future Vision and Roadmap of Organic and Molecular Electronics/Bioelectronics, KAJI H et al., Special Program Symposium, "Future Vision of the Japan Society of Applied Physics–Academic Roadmap toward 2040", The 55th Annual Meeting of the Japan Society of Applied Physics, Chiba, Japan, 28 March 2008.

Phase Separation Behavior of Aqueous Suspensions of Tunicate Cellulose Nanofibers Prepared by HCl Hydrolysis and TEMPO-Mediated Oxidation, Hirai A, Iwata D, Horii F, Nomura A, Tsujii Y, Tsuji M, 15th Annual Meeting, Cellulose Soc., Japan, Kyoto, 10 July 2008.

Grants

Kaji H, Synthesis of Novel Organic Electroluminescence Materials and the Application for Organic Devices, Research for Promoting Technological Seeds, Japan Science and Technology Agency (JST), 9 July 2008–13 March 2009.

Kaji H, Science and Functions of Organic Amorphous Materials, Grant-in-Aid for Scientific Research (A), 1 April 2005–31 March 2008.

Kaji H, Electronic State Analysis of Organic Photoelectric Conversion Systems by Quantum Chemical Calculation and Nuclear Magnetic Resonance, Grant-in-Aid for

Organic Light-Emitting Diodes Fabricated from Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) in Different Crystalline Polymorphs

Tris(8-hydroxyquinoline) aluminum(III) (Alq_3) has been one of the most widely used light-emitting electron-transport materials in organic lights emitting diodes (OLEDs). It is known that there are four polymorphs, α, β, γ, and δ forms, in crystalline Alq_3 and that they show green or blue luminescence under UV-irradiation depending on their isomeric states (see Figure 1). However, their relationships with the performance of OLEDs have not been investigated.

We prepared three kinds of Alq_3 crystals, α-Alq_3, δ-Alq_3, and mixture of α, γ, δ-Alq_3, by temperature gradient sublimation and thermal annealing. The crystals show different colors under UV-irradiation as shown in Figure 1. By evaporating each crystal under vacuum, three OLEDs with the configuration of ITO / NPD 40nm / Alq_3 60 nm / Cs_2CO_3 / Al were fabricated. All the devices exhibit yellowish-green electroluminescence (EL) emissions, irrespective of the polymorphs before the vacuum evaporation. However, the three devices show different EL performances as shown in Figure 1. The current efficiency of the device fabricated from the mixture of α, γ, δ-Alq_3 is larger than the other two devices fabricated from α-Alq_3 and δ-Alq_3. We carried out the same experiments several times to confirm the reproducibility. The enhancement factors slightly change, but the current efficiencies of the three devices are always in the order of α, γ, δ-Alq_3 > δ-Alq_3 ≧ α-Alq_3.

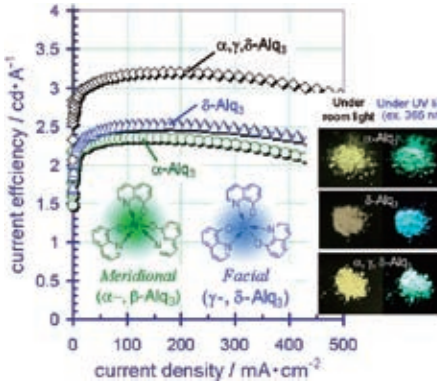


Figure 1. Current efficiency-current density characteristics for the OLEDs fabricated from three kinds of Alq_3 crystals; α-Alq_3, δ-Alq_3, and the mixture of α, γ, δ-Alq_3.

Charge Transport Paths in Organic Solids, *N,N'*-diphenyl-*N,N'*-di(*m*-tolyl) Benzidine (TPD)

Charge transports in organic materials are of immense interest for device applications such as OLEDs. For OLEDs, *N,N'*-diphenyl-*N,N'*-di(*m*-tolyl)benzidine (TPD) is widely used as a hole-transport material. We investigated the paths for charge transports in the orthorhombic and monoclinic polymorphs of TPD. Based on Marcus theory, we calculated charge transfer rate constants for all the neighboring molecular pairs in both polymorphs by density functional theory (DFT) method. The electron transfer rate constants were less than 3×10^{11} s^{-1} for any pairs in both polymorphs, due to its large reorganization energy for electron transfer. In contrast, the small reorganization energy for hole transfer resulted in large hole transfer rate constants. Moreover, percolation paths were found for hole transfer with large rate constants in both polymorphs. In the orthorhombic polymorph, the paths are along the c axis with the hole transfer rate constant of 5×10^{12} s^{-1} (Figure 2). In the monoclinic polymorph, holes can be transported in various directions with the rate constants of 2×10^{12}–4×10^{12} s^{-1} (Figure 3). In addition to the small reorganization energy and the large charge transfer integrals, the existence of percolation paths is found to be a crucial factor for high carrier-transport property.

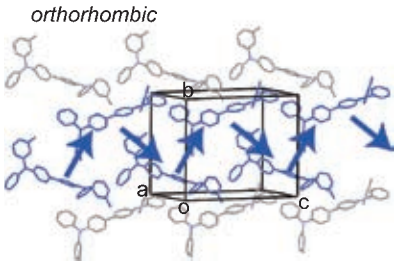


Figure 2. Hole transport paths in the orthorhombic polymorph of TPD.

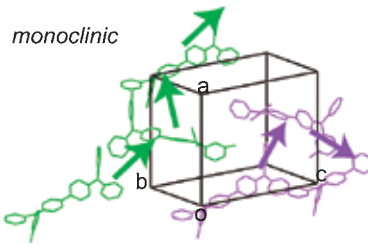


Figure 3. Hole transport paths in the monoclinic polymorph of TPD.

Scientific Research on Priority Areas, 1 April 2007–31 March 2008.

Hirai A, Structure Control of Native Polymer Nano-Assemblies by Magnetic Field, Grant-in-Aid for Scientific Research, 1 April 2007–31 March 2010.

Division of Environmental Chemistry
- Hydrospheric Environment Analytical Chemistry -

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

Prof
SOHRIN, Yoshiki
(D Sc)

Assoc Prof
UMETANI, Shigeo
(D Sc)

Assist Prof
NORISUYE, Kazuhiro
(D Sc)

Assist Prof*
FIRDAUS, Mochamad Lutfi
(D Sc)

Techn
MINAMI, Tomoharu
(D Eng)

* Division of Environmental Chemistry, Laboratory of Trace Elemental Tomography

Lecturer (pt)

NORIKI, Shinichiro (D Fish Sc)
Graduate School of Environmental Science, Hokkaido University

Students

NAKAGAWA, Yusuke (D2)
ABIGAIL, Parcasio Cid (D1)
HIGO, Eri (M2)
NISHIDA, Shinsuke (M2)
OKABE, Taro (M2)
SATO, Kengo (M1)
TANIGAWA, Masahito (M1)

Visitor

Prof LI, Yuan-Hui University of Hawaii, USA, 24–29 April 2008

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 paleoocean.

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

Research Activities (Year 2008)

Publications

Sohrin Y, Urushihara S, Nakatsuka S, Kono T, Higo E, Minami T, Norisuye K, Umetani S: Multielemental Determination of GEOTRACES Key Trace Metals in Seawater by ICPMS after Preconcentration Using an Ethylenediaminetriacetic Acid Chelating Resin, *Anal. Chem.*, **80**, 6267-6273 (2008).

Lai X, Norisuye K, Mikata M, Minami T, Bowie AR, Sohrin Y: Spatial and Temporal Distribution of Fe, Ni, Cu and Pb along 140°E in the Southern Ocean during Austral Summer 2001/02, *Mar. Chem.*, **111**, 171-183 (2008).

Kurahashi K, Umetani S, Sohrin Y: Solvent Extraction of Divalent Metal Ions with Azacrown Ether Substituted Acylpyrazolones, *Anal. Sci.*, **24**, 225-229 (2008).

Presentations

Multielemental Determination of GEOTRACES Key Trace Metals by Column Concentration and ICP-MS, Norisuye K, Urushihara S, Nakatsuka S, Kono T, Higo E, Minami T, Sohrin Y, 18th Annual V.M. Goldschmidt Conference, 14 July 2008.

Precise Mo Isotopic Analysis on Pacific and Antarctic Seawater, Nakagawa Y, Firdaus ML, Norisuye K, Sohrin Y, Irisawa K (Tokyo Institute of Technology), Hirata T (Tokyo Institute of Technology), 18th Annual V.M. Goldschmidt Conference, 14 July 2008.

Behaviors of Incompatible Elements in the Western North Pacific Ocean, Firdaus ML, Nakagawa Y, Norisuye K, Sohrin Y, 18th Annual V.M. Goldschmidt Conference, 15 July 2008.

Design of Extraction Reagents of High Selectivity Based on Steric Factors, Umetani S, Fukui Y, Uezu K (University of Kitakyushu), International Solvent Extraction Conference, 16 September 2008.

Multielemental Determination of the Bioactive Trace Metals in Seawater by Solid Phase Extraction-ICPMS and Its Application to the Bering Sea

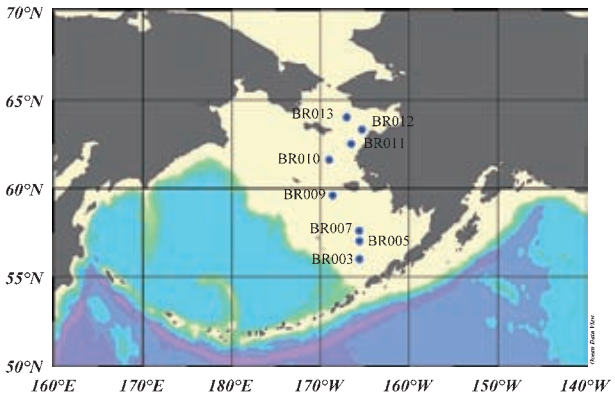


Figure 1. Location of stations.

The temporal and spatial distributions of trace metals in seawater are controlled by biological, chemical and physical processes. Al, Mn, Fe, Co, Ni, Cu, Zn, Cd and Pb, which are referred to as bioactive trace metals, strongly influence marine organisms. Since direct determination of these metals is not possible due to the very low concentrations and the interference from major ions, it is necessary to separate and concentrate them. Solid phase extraction with chelating absorbents, such as iminodiacetic acid chelating resin (Chelex 100), vinyl polymer resin-immobilized 8-hydroxyquinoline (TSK-8HQ), fluorinated metal alkoxyde glass-immobilized 8-hydroxyqunoline (MAF-8HQ), have been widely used for the preconcentration. However, it is difficult for these adsorbents to collect Mn quantitatively and to remove alkali and alkaline earth metals. We have developed a preconcentration method of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd and Pb from seawater using a novel chelating resin with ethylendiaminetriacetic acid group, NOBIAS CHELATE-PA1 (Hitachi High-Technologies Co. Ltd.), packed in PFA tubes.[(1)] This is the unique method that realize the quantitative collection of these metals without contamination and the removal of alkali and alkaline earth metals. We applied this method to elucidate the spatial distribution of trace metals in the Bering Sea.

The Bering Sea, which is located between the Aleutian Islands and the Bering Strait, has continental shelf in the eastern area and a deep basin in the western area. The eastern area shows the highest biological productivity in the world, whereas the western area is characterized by high-nutrient low-chlorophyll. Seawater samples were collected from 8 stations in the eastern Bering Sea during the MR00-K06 cruse of R/V Mirai using a CTD carousel on which Niskin-X samplers were mounted (Figure 1). Filtered and unfiltered seawater samples were acidified to pH 2.2 with HCl. These were used for the determination of dissolved (D) and acid-dissolvable (AD) metals, respectively.

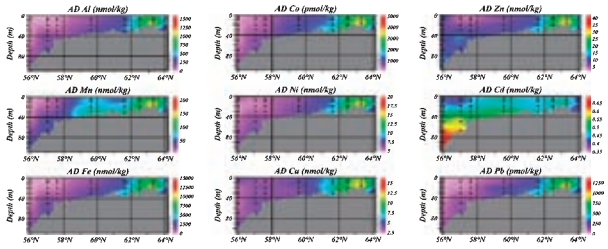


Figure 2. Sectional distributions of acid dissolvable trace metals in the Bering Sea.

Figure 2 shows the sectional distribution of AD species. The AD species include D and labile particulate species (such as those adsorbed onto iron oxyhydroxides and clay minerals, and those incorporated into organisms) which dissolve during storage. The concentrations of the AD species are high at BR011 and 012. These stations are located near the estuary of the Yukon River, where salinity was low because of the inflow of the river water. Therefore, the AD species should be supplied by the river. AD-Cd showed maximum above the bottom of BR003 and 005. The concentration of chlorophyll *a* was highest in surface water at BR005 among all stations. Therefore, it is likely that Cd was taken up by phytoplankton, precipitated with sinking particles, and remineralized in the depth.

[1] Y. Sohrin *et al.*, *Anal. Chem.*, **80**, 6267 (2008).

Grants

Sohrin Y, Development of Redox Proxy Using Molybdenum and Tungsten and Reconstruction of Environmental Changes in the Japan Sea, Challenging Exploratory Research, 1 April 2008–31 March 2010.

Norisuye K, Development of a Method for Determination of Divalent Iron and Elucidation of the Behavior in the Ocean, Steel Industry Foundation for the Advancement of Environmental Protection Technology, 1 November 2007–31 October 2009.

Division of Environmental Chemistry
- Solution and Interface Chemistry -

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

Prof
NAKAHARA, Masaru
(D Sc)

Assoc Prof
MATUBAYASI, Nobuyuki
(Ph D)

Assist Prof
WAKAI, Chihiro
(D Sc)

PD
PURQON, Acep
(D Sc)

PD
WANG, Jianyi
(Ph D)

Students

YASAKA, Yoshiro (D2)
KIMURA, Hiroshi (M2)
SHINTANI, Megumi (M2)
IYUKU, Hiroomi (M1)
MIYA, Shingo (M1)

Visitor

VACHA, Robert Czech Academy of Science, Czech Republic, 9 November–20 December 2008

Scope of Research

The structure, dynamics, and reaction of solutions with fine tunability and/or with nano-scale inhomogeneity are investigated by NMR spectroscopy, computer simulation, and statistical-mechanical theory of solutions. Solvation is systematically elucidated for ionic liquids and supercritical fluids from both the static and dynamic viewpoints, and non-catalytic reactions of environmental importance are developed. The structural organization and fluctuation and the molecular binding are investigated for soft, self-organizing systems such as micelle, protein, and lipid membrane.

Research Activities (Year 2008)

Publications

Giordani C, Wakai C, Yoshida K, Okamura E, Matubayasi N, Nakahara M: Cholesterol Location and Orientation in Aqueous Suspension of Large Unilamellar Vesicles of Phospholipid Revealed by Intermolecular Nuclear Overhauser Effect, *J. Phys. Chem. B*, **112**, 2622-2628 (2008).

Matubayasi N, Shinoda W, Nakahara M: Free-energy Analysis of the Molecular Binding into Lipid Membrane with the Method of Energy Representation, *J. Chem. Phys.*, **128**, 195107 (13 pages) (2008).

Presentations

Free-Energy Analysis of Nano-Organized Systems in Solution, Matubayasi N, The 2nd International Symposium on "Molecular Theory for Real Systems", Okazaki, Japan, 4–6 August 2008.

High-Temperature Multinuclear-Magnetic-Resonance Probe for the Analysis of Structure, Dynamics, and Chemical Reactions in Supercritical Water, Nakahara M, The 15th International Conference on the Properties of Water and Steam, Berlin, Germany, 7–11 September 2008.

Grants

Nakahara M, Free-Energy Analysis of Nanoscale, Molecular Aggregates with the Method of Energy Representation, Next-Generation Integrated Nanoscience Simulation Software Project, 1 April 2008–31 March 2013.

Matubayasi N, Informational Coarse-Graining Models of Biomolecules and their Interactions, Japan Science and Technology Agency, 1 October 2007–31 March 2012.

Matubayasi N, Free-Energy Analysis of Molecular Binding into Membrane in the Method of Energy Representation, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Wakai C, NMR Study on Dynamics of Water Molecule, Organic Molecules, and Ions in Ionic Liquids, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2010.

Award

Matubayasi N, Award for Distinguished Achievement and Nose Memorial Award, The Japan Society of Molecular Simulation, 18 November 2008.

Free-Energy Analysis of Molecular Binding into Lipid Membrane

The lipid membrane distinguishes one side of the solution from the other, and plays important roles in distribution and transport of a molecule. A key quantity to govern the membrane function is the free energy of molecular binding. We have established a new and fast scheme of free-energy calculation for the molecular binding in membrane by combining a new theory of solutions with molecular simulation. The new theory is called the method of energy representation, and expresses the free energy in solution in terms of the information of the intermolecular interaction energy. It accelerates the free-energy calculation by several tens time faster than the conventional methods, and nano-inhomogeneous solutions such as micelle and membrane is now well within the scope of all-atom calculation.

Figure 1 shows the free energy $\Delta\mu$ of binding of hydrophobic solute into DMPC (1,2-dimyristoyl-*sn*-glycero-3-phosphatidylcholine) bilayer. A hydrophobic solute is free-energetically stabilized within the membrane inside compared to bulk water. The stability is quite high even in the polar and hydrophilic headgroup region. This is due to the interaction with water present outside the membrane; the effect of excluded volume, which is the source of hydrophobicity, reduces drastically in the interfacial region, while the medium-range attraction by dispersion interaction persists. Corresponding experimental information, especially in the headgroup region, is now being obtained. It is also possible to calculate the membrane-water partition coefficient from Figure 1. This is a good step toward material design using soft, lipid membranes.

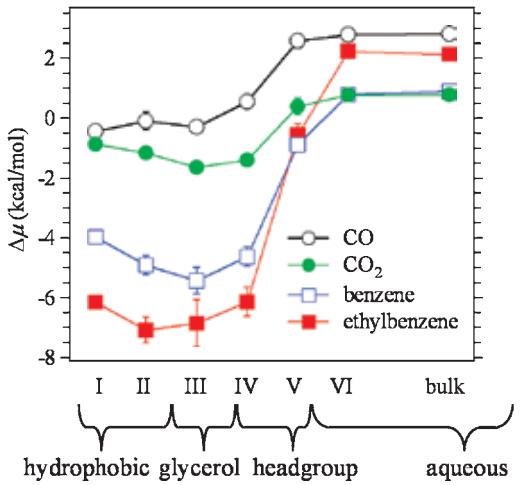


Figure 1. The free-energy change $\Delta\mu$ of inserting a hydrophobic solute into DMPC membrane. Six regions are introduced with an interval of 5 Å and are numbered I....VI from the membrane inside to outside.

Water as an In-Situ NMR Indicator for Impurity Acids in Ionic Liquids

Molten salts which have relatively low melting points are called ionic liquids (ILs). ILs are attracting much interest as environmentally-friendly, new and unique reaction medium. In investigating the solvent effect of ILs, it is important to establish an analytical method to certify the purity of ILs studied. Acids can be the most detrimental impurity to the reaction study due to its catalytic activity. Although titration and electrochemical methods are popular in aqueous systems, they are not sufficiently sensitive when applied to ILs.

In the present work, we have developed a sensitive in-situ NMR spectroscopic analysis method for the detection of impurity acids contained in ionic liquids (ILs). The chemical shift of water dissolved into the tested IL was used to measure the impurity level. Water was adopted as the impurity indicator, and its chemical shift changes with the concentration of the coexisting acid through proton exchange. Owing to the high resolution power of NMR, the detection limit is below the level of 10^{-3} mol kg^{-1}. A new method is applicable to a number of commonly used ILs such as the imidazolium- and ammonium-based ILs except for those composed of acidic cations or anions.

The method was utilized to monitor the purification efficiency in the recrystallization of a typical hydrophilic IL, 1-butyl-3-methylimidazolium methanesulfonate from acetone. As seen in Figure 2, the chemical shift of water was drastically changed before and after the recrystallization. It was demonstrated that impurity acids can be almost perfectly removed by single or double recrystallization.

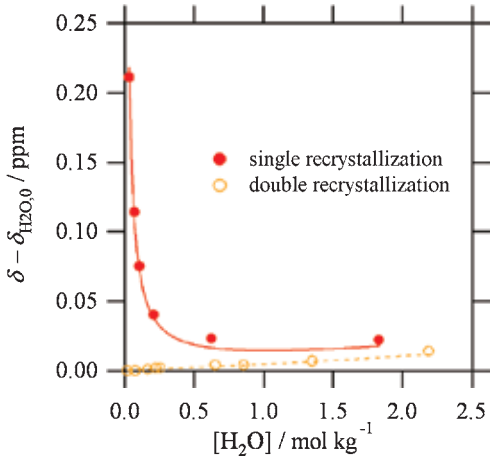


Figure 2. Plots of the chemical shift (δ-$\delta_{H2O,0}$) against [H_2O] for [bmim]$^+$[CH_3SO_3]$^-$ after single (filled circles) and double (open circles) recrystallization. The $\delta_{H2O,0}$ is the chemical shift of water in the acid-free ionic liquid in the limit of [H_2O] = 0. The ionic liquid after only single recrystalization contains the impurity acid at 1.8 mmol kg^{-1}, whereas that after double recrystallization can be regarded as perfectly pure.

Division of Environmental Chemistry
- Molecular Microbial Science -

http://www.kuicr.kyoto-u.ac.jp/labos/bm2/Pages/lab.html

Prof
ESAKI, Nobuyoshi
(D Agr)

Assoc Prof
KURIHARA, Tatsuo
(D Eng)

Assist Prof
MIHARA, Hisaaki
(D Agr)

Proj Res*
KAWAMOTO, Jun
(D Agr)

PD
KUROKAWA, Suguru
(D Agr)

Res Associates (pt)

OMORI, Taketo
YAMAUCHI, Takae
TANAKA, Yumi

Technicians (pt)

KITAYAMA, Kaori
UTSUNOMIYA, Machiko

Students

JITSUMORI, Keiji (D3)
TOBE, Ryuta (D3)
AMR, Mohammed Hassan (D2)
ZHANG, Wanjiao (D2)
FUKUYAMA, Sadanobu (D1)
HIDESE, Ryota (D1)
KOGA, Keitaro (M2)
HIRUTA, Satoko (M2)
HONDA, Ai (M2)
PARK, Jungha (M2)
SATO, Sho (M2)
IMAI, Takeshi (M1)
KASAI, Wataru (M1)
MOMOKAWA, Yusuke (M1)
DAI, Xianzhu (RS)
VASUDEVAN, Anoop (RS)
WANG, Yu (RS)

*Assist Prof of Institute of Sustainability Sience

Visitor

Prof JHEE, Kwang-Hwan Department of Applied Chemistry, Kumoh National Institute of Technology, Korea, 27 February 2008–17 February 2009

Scope of Research

Structures and functions of biocatalysts, in particular, pyridoxal enzymes and enzymes acting on xenobiotic compounds, are studied to elucidate the dynamic aspects of the fine mechanism for their catalysis in the light of recent advances in gene technology, protein engineering and crystallography. In addition, the metabolism and biofunction of sulfur, selenium, and some other trace elements are investigated. Development and application of new biomolecular functions of microorganisms are also studied to open the door to new fields of biotechnology. For example, cold-adaptation mechanism and applications of psychrotrophic bacteria are under investigation.

Research Activities (Year 2008)

Presentations

Sulfur Trafficking in Biosynthesis of Iron-Sulfur Cluster, Mihara H, International Symposium on Chemistry of Reductases, 11 March 2008.

Physiological Role of Eicosapentaenoic acid in a Psychrotroph *Shewanella livingstoensis* Ac10, Esaki N, Kawamoto J, Sato S, Kurihara T, Hosokawa M, Baba T, Sato SB, 3rd International Conference on Polar and Alpine Microbiology, 11 May 2008.

Cold-adaptation Mechanisms and Applications of an Antarctic Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, Kurihara T, Esaki N, TBIT's 1st Annual World Congress of ibio-2008, 19 May 2008.

Enzyme Engineering and Microbial Technology for Biocatalysis, Esaki N, 2008 International Symposium and Annual Meeting, 26 June 2008.

A Novel Flavoenzyme Involved in Bacterial Metabolism of 2-Chloroacrylate, Kurihara T, Mowafy A M, Fujita M, Kurata A, Esaki N, 4th Japan-Finland Biotechnology Symposium, 2 October 2008.

Grants

Esaki N, Investigation of Organisms Carrying a Unique Selenium Metabolism and Its Application to Bioremediation, Grant-in-Aid for Scientific Research (B), 1 April 2006–31 March 2008.

Esaki N, Structure-Function Analysis of Selenium-specific Chemical Conversion System and Co-translational Insertion of Selenium into Protein, Grant-in-Aid for Scientific Research (B), 1 April 2007–31 March 2009.

Enzymatic Synthesis of (*S*)-2-Chloropropionate by Asymmetric Reduction of 2-Chloroacrylate with 2-Haloacrylate Reductase Coupled with Glucose Dehydrogenase

Asymmetric reduction of carbon-carbon double bonds is one of the most widely used methods for the production of chiral compounds useful as pharmaceuticals, agrochemicals, and so on. Accordingly, enzymes catalyzing this type of reaction have been attracting a great deal of attention from the industrial point of view. We found a novel NADPH-dependent enzyme catalyzing the asymmetric reduction of a carbon-carbon double bond of 2-haloacrylate from 2-chloroacrylate (2-CAA)-assimilating bacterium, *Burkholderia* sp. WS. The enzyme, named 2-haloacrylate reductase, catalyzes the stereospecific conversion of 2-chloroacrylate into (*S*)-2-chloropropionate ((*S*)-2-CPA), which is useful as a chiral synthon for the synthesis of phenoxypropionic acid herbicides. (*S*)-2-CPA is synthesized by optical resolution of a racemic mixture of 2-chloropropionate by a conventional method, in which (*R*)-2-chloropropionate of a racemic mixture is selectively degraded with (*R*)-2-haloacid dehalogenase. However, the theoretical maximum yield of this method is 50%, and a new procedure for the production of (*S*)-2-CPA superior to the conventional method in terms of conversion yield is expected. We constructed a system for asymmetric reduction of 2-CAA to produce (*S*)-2-CPA with recombinant *Escherichia coli* cells producing 2-haloacrylate reductase from *Burkholderia* sp. WS and glucose dehydrogenase from *Bacillus subtilis* for regeneration of NADPH (Figure 1). The system provided 37.4 g/*l* (*S*)-2-chloropropionate in more than 99.9% *e.e.*

The *iscS* Gene Deficiency Affects the Expression of Pyrimidine Metabolism Genes

Inactivation of *iscS* encoding cysteine desulfurase results in a slow growth phenotype associated with the deficiency of iron–sulfur clusters, thiamine, NAD, and tRNA thionucleosides in *Escherichia coli*. By using differential screening strategies, we identified 2 pyrimidine salvage enzymes, namely, uridine phosphorylase and cytidine deaminase, which were down-regulated in the *iscS* mutant (Figure 2). Both enzymes are positively regulated by the cAMP receptor protein. We also identified a novel protein complex, namely, YeiT–YeiA, whose expression level was decreased in the *iscS* mutant. The recombinant YeiT–YeiA complex exhibited NADH-dependent dihydropyrimidine dehydrogenase activity, indicating its role in pyrimidine metabolism. These results provide a clue to the possible role of *iscS* in pyrimidine metabolism by gene regulation.

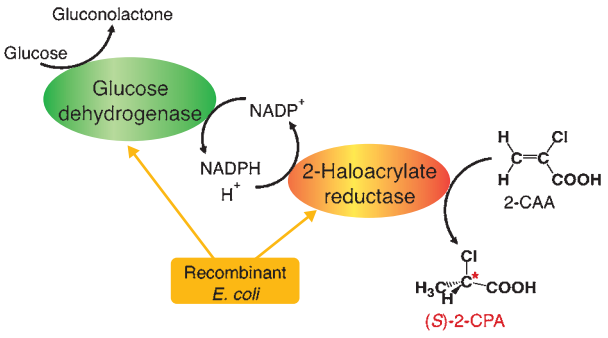


Figure 1. Enzymatic synthesis of (*S*)-2-chloropropionate by asymmetric reduction of 2-chloroacrylate with 2-haloacrylate reductase coupled with glucose dehydrogenase.

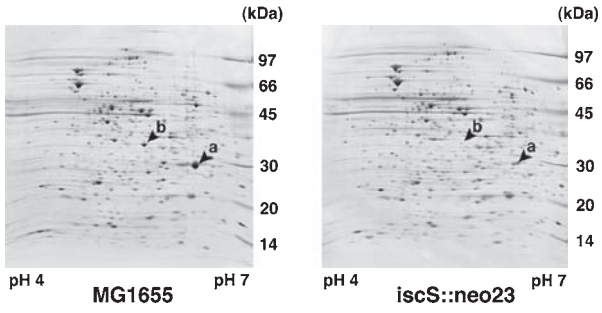


Figure 2. 2-Dimensional electrophoresis of crude extracts of MG1655 (left panel) and iscS::neo23 (right panel).

Kurihara T, Exploration of Novel Cold-adapted Microorganisms to Develop a System for the Production of Useful Compounds at Low Temperatures, Grant-in-Aid for Scientific Research (B), 1 April 2007–31 March 2009.

Kurihara T, Analysis of the Molecular Basis for Cold Adaptation of Psychrotrophic Bacteria, Grant-in-Aid for Scientific Research (B), 1 April 2008–31 March 2011.

Mihara H, Studies on Mechanism of Selenium-specific Recognition and Selenoprotein Biosynthetic Machinery, Grant-in-Aid for Young Scientists (B), 1 April 2006–31 March 2008.

Division of Multidisciplinary Chemistry
- Polymer Materials Science -

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

Prof
KANAYA, Toshiji
(D Eng)

Assoc Prof
NISHIDA, Koji
(D Eng)

Assist Prof
MATSUBA, Go
(D Eng)

Students

RAHMAN, Nelly (D3)
ASAKAWA, Harutoshi (D1)
ITO, Chie (M2)
OKADA, Kazuma (M2)
TANAKA, Kentaro (M2)
TOMOHISA, Hiroshi (M2)
KAWABATA, Jun (M1)
KAWASHIMA, Kazuko (M1)
MORITA, Hideyuki (M1)
ZHAO, Yunfeng (M1)
ANADA, Ryota (UG)
MATSUI, Kazuya (UG)
MATSUI, Tamito (UG)
MATSUMOTO, Norihiro (UG)
TERATANI, Makoto (UG)

Visitors

Prof MUKHERJEE, Manabendra — Saha Institute of Nuclear Physics, India, 17–29 March 2008 / 2–14 December 2008
Prof GABRYS, Barbara J — University of Oxford, UK, 12–30 May 2008

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 the glassy or molten state to spherulites; the dynamics in disordered polymer materials including low-energy excitation or excess heat capacity at low temperatures, glass transition and local segmental motions; formation processes and structure of polymer gels; the structure and molecular motion of polyelectrolyte solutions; the structure of polymer liquid crystals.

Research Activities (Year 2008)

Publication

Ogawa H, Kanaya T, Nishida K, Matsuba G: Composition Fluctuations before Dewetting in Polystyrent/Poly(vinyl methyl ether) Blend Thin Films, *Polymer*, **49**, 2553-2559 (2008).

Presentations

Temperature Effects on Poly (L-lactic acid) Crystallization, Uchida H, Kawai T, Rahman N, Matsuba G, Nishida K, Kanaya T, The 57th SPSJ Annual Meeting, Yokohama, 28–30 May 2008.

Rapid Temperature Jump Stage for Optical Microscope, Nishida K, The Polymer Processing Society 24th Annual Meeting, Salerno, Italy, 15–19 June 2008.

Structure Formation of Polyethylene under Drawing with Small Angle Neutron Scattering Measurements, Ito C, Matsuba G, Nishida K, Kanaya T, 17th Autumn Meeting in Combined Societies about Fibers in Japan, Nara, 28–29 August 2008.

Effects of Surface Flatness of Glass Substrates on the Orientation and Size of the Grains of Colloidal Crystals Obtained by Centrifugation, Asakawa H, Suzuki Y, Summer Seminar of Society of Fiber Science and Technology in Japan, Oumi-hachiman, 10–12 September 2008.

Inelastic Neutron Scattering from Polystyrene Thin Films, Kanaya T, Advances in Polymer Science & Neutron Scattering, London, UK, 14–15 September 2008.

Crystallization Process of Polyesters under Shear Flow, Tomohisa H, Matsuba G, Nishida K, Kanaya T, The 57th SPSJ Discussion (Autumn) Meeting, Osaka, 24–26 September 2008.

Annealing of Mesomorphic Phase of Isotactic Polypropylene, Okada K, Nishida K, Matsuba G, Konishi T, Kanaya T, The 57th SPSJ Discussion (Autumn) Meeting, Osaka, 24–26 September 2008.

Critical Dissolution Ionic Strength of Aqueous Chito-

Precursor of Shish-kebab in Isotactic Polystyrene under Shear Flow

The polarized optical microscope (POM), depolarized light scattering (DPLS) and small-angle X-ray scattering measurements were performed on the structure formation process or the crystallization process of isotactic polystyrene (iPS) under shear flow below and above the nominal melting temperature T_m. It was found that an anisotropic oriented structure termed here as a string-like object was formed in μm scale even above the nominal melting temperature and stable for more than 24 hours, but melted at around 270 °C far above T_m in Figure 1. The string-like object acts as a nucleation agent for the folded chain lamella crystal (or the kebab), and was assigned to a precursor of the shish-kebab from small angle x-ray scattering measurements. Based on the results we have discussed two possible structures for the string-like object: one is fringed micelle type structure including partially extended chain crystals and the other is liquid crystal-like structure formed through extended network of entangled polymer chains.

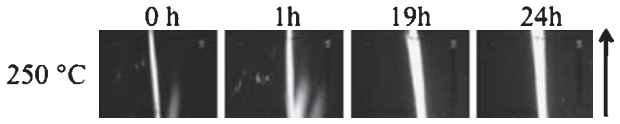


Figure 1. Time evolution of POM pictures of iPS during the annealing process at various temperatures after applying a pulse shear with shear rate $30s^{-1}$ and shear strain 12000 % at 250 °C up to 24 h. Note that the nominal melting temperature of iPS is 223 °C.

Heterogeneous Dynamics of Polymer Thin Films

In the last decade many studies have been performed on polymer thin films to reveal very interesting but unusual properties. One of the most interesting findings is that the glass transition temperature T_g decreases with film thickness in the thickness range below about 400 Å. It is believed that one of the most important key issues to solve the unusual properties of polymer thin films is heterogeneous dynamics of polymer thin films [1]. We therefore studied the dynamic heterogeneity of polystyrene thin films in glassy state in terms of non-Gaussian parameter A_0, which is a measure of dynamic heterogeneity, using inelastic neutron scattering [2]. It was found that the non-Gaussian parameter increased with decreasing the film thickness, suggesting the increase in the dynamic heterogeneity. Assuming a simple two layer model consisting of an interface hard layer and a bulk-like layer we analyzed the thickness dependence of the non-Gaussian parameter A_0 and the mean square displacement $\langle u^2 \rangle$ to find that the hard layer has the thickness of ~130 Å and the mean square displacement of ~0.018 $Å^2$ at 230 K as shown in Figures 1 and 2, suggesting dynamic heterogeneity of polymer thin films.

[1] Inoue R, Kanaya T, Nishida K, Tsukushi I, Shibata K, *Phys. Rev.* E**77**, 032801-1-032801-4 (2008).
[2] Inoue R, Kanaya T, Nishida K, Tsukushi I, Taylor J, Levett S, *Eur. Phys. J.,* E **24**, 55-60 (2007).

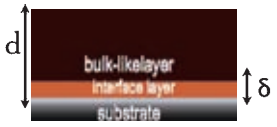


Figure 2. Schematic representation of two layer model

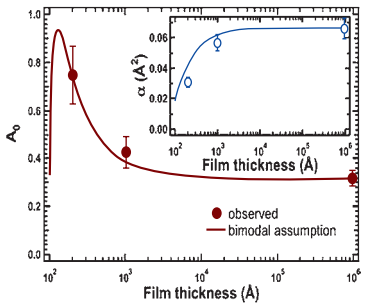


Figure 3. Non-Gaussian parameter A_0 at 230 K as a function of film thickness. Inset shows mean square displacement $\langle u^2 \rangle$. Solid curves are the results of fits with two layer model.

san, Tanaka K, Nishida K, Gabrys BJ, Lawrence MJ, Kanaya T, The 57th SPSJ Discussion (Autumn) Meeting, Osaka, 24–26 September 2008.

Formation Process of Shish-kebab Structure under Shear Flow, Matsuba G, The 3rd International Symposium on Polymer Science (NIST-JAPAN), Nagoya, 10–11 November 2008.

Distribution of Glass Transition Temperature in Polystyrene Multilayered films, Kawashima K, Inoue R, Matsuba G, Nishida K, Kanaya T, IUMRS-ICA, Nagoya, 9–14 December 2008.

Grants

Kanaya T, Higher Order Structure Formation in Induction Period of PLA Crystallization and External Fields, Collaboration Research with Toyota Motor Corporation and Toyota CRDL., INC, 15 January 2003–30 September 2009.

Nishida K, Kanaya T, Matsuba G, Control of Higher Order Structure by Crystallization via Mesomorphic Phase, Grant-in-Aid for Scientific Research (C), 1 April 2007–31 March 2009.

Matsuba G, Correlation between Phase Separation and Crystallization of Polyolefins, Grant-in-aid for Young Scientists (B), 1 April 2007–31 March 2009.

Division of Multidisciplinary Chemistry
- Molecular Rheology -

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

Prof
WATANABE, Hiroshi
(D Sc)

Assoc Prof
MASUBUCHI, Yuichi
(D Eng)

Assist Prof
MATSUMIYA, Yumi
(D Eng)

Program-Specific Assist Prof
UNEYAMA, Takashi
(D Sc)

Techn
OKADA, Shinichi

Students

TAKAHASHI, Hideaki (D3)
FURUICHI, Kenji (D2)
CHEN, Quan (D2)
HORIO, Kazushi (D1)
YAOITA, Takatoshi (D1)
MISHIMA, Eri (M2)
SUZUKI, Takeshi (M2)
TANAKA, Satoshi (M2)
KAWAKITA, Hiroshi (M2)
KINOSHITA, Taro (M2)
MORIYA, Motoaki (M2)
SAITO, Ryo (M1)
UNO, Akiko (M1)
HIRAMOTO, Keisuke (UG)
KATAKURA, Shiro (UG)

Guest Res Assoc

RAKKAPAO, Natthida (RS)

Visitors

Prof MARRUCCI, Giuseppe	Università degli studi di Napoli "Federico II", Italy, 15 March–15 April 2008
Prof SCHIEBER, Jay	Illinois Institute of Technology, USA, 17–30 March 2008
Prof IANNIRUBERTO, Giovanni	Università degli studi di Napoli "Federico II", Italy, 1–7 June 2008
Prof KORNFIELD, Julia	California Institute of Technology, USA, 1–9 June 2008
Prof LIGOURE, Christian	University of Montpelier, France, 1–13 June 2008
LEE, Ayoung	Seoul National University, Korea, 25 March–28 August 2008
ROSCHZTTARDTZ, Frederico	University of Leeds, UK, 21 May–25 November 2008

Scope of Research

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

Research Activities (Year 2008)

Publications

Chen Q, Matsumiya Y, Masubuchi Y, Watanabe H, Inoue T: Component Dynamics in Polyisoprene/Poly(4-tert-butylstyrene) Miscible Blends, *Macromolecules,* **41(22)**, 8694-8711 (2008).

Masubuchi Y, Watanabe H, Ianniruberto G, Greco F, Marrucci G: Comparison among Slip-Link Simulations of Bidisperse Linear Polymer Melts, *Macromolecules*, **41(21)**, 8275-8280 (2008).

Watanabe H, Matsumiya Y, van Ruymbeke E, Vlassopoulos D, Hadjichristidis N: Viscoelastic and Dielectric Relaxation of a Cayley-Tree-Type Polyisoprene: Test of Molecular Picture of Dynamic Tube Dilation, *Macromolecules,* **41**, 6110-6124 (2008).

Presentations

Dielectric and Viscoelastic Investigation of Entanglement Relaxation, Watanabe H, 2008 APS March Meeting, New Orleans, 13 March 2008 (Invited).

Molecular Simulations of Polymers with Primitive Chain Network Model, Masubuchi Y, MSSMBS2008, 12 September 2008, Dubna, Russia (keynote, invited).

Viscoelastic and Dielectric Relaxation of a Cayley-Tree Type Polyisoprene: Test of Molecular Picture of Dynamic Tube Dilation

We have experimentally elucidated that entangled polymer chains with multi-branched structure relax through the constraint release mechanism. This result provided us with significant progress in our understanding of entanglement dynamics.

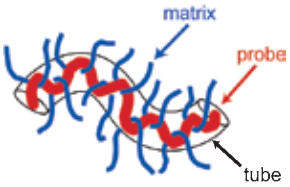


Figure 1. Schematic illustration of tube model.

The entanglement between polymer chains strongly affects the global (large scale) thermal motion of the chains governing their flow behavior. In the widely utilized tube model (cf. Figure1), the entanglement effect for a focused chain (probe) is represented by a tube along the probe backbone formed by the surrounding chains (matrix) and the probe motion is constrained in this tube. The current tube model incorporates fluctuation of the probe length measured along the tube axis as well as the removal/reformation of the tube wall resulting from motion of the tube-forming matrix chains. The probe motion activated by this wall removal/reformation, referred to as the *constraint release* (CR) motion, represents the motional cooperativity of the chains within the context of the mean-field tube model. On an increase of the time scale of observation, the effective tube dilates as a result of the CR motion. The current tube model regards the relaxed portion of the chains as a simple solvent to evaluate the diameter of the dilated tube. This model describes the viscoelastic data of polymers well, but the validity of the model for the chain dynamics itself remains unclear.

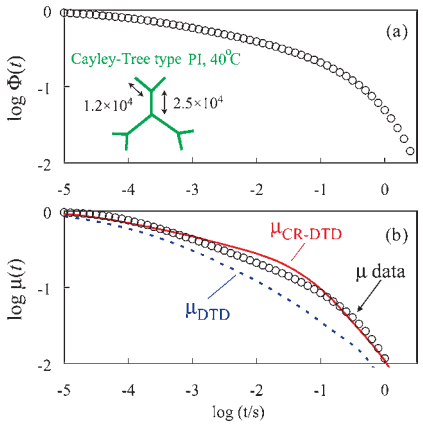


Figure 2. Dielectric relaxation function (a) and viscoelastic relaxation function (b) of Cayley-tree cis-polyisoprene.

For this problem, we focused on a fact that the viscoelastic and dielectric relaxation functions, $\mu(t)$ and $\varphi(t)$, of chains having the type-A electrical dipoles (parallel along the chain backbone) detect the same global motion with different averaging moments to formulate a relationship of these functions, $\mu_{DTD}(t) = \{\varphi(t)\}^d$ + minor contribution from fluctuation at tube edge (d = 1-1.3), that should hold if the relaxed portion is equivalent to the simple solvent. They tested this relationship for a representative multi-branched chain having the type-A dipoles, a Cayley-tree *cis-polyisoprene (CT-PI), to find that the above relationship does not hold for the* $\mu(t)$ and $\varphi(t)$ data of CT-PI and thus the relaxed portion is not equivalent to the solvent. This result demonstrated that the widely utilized, current tube model includes a flaw. Furthermore, we derived the other type of $\mu(t)$-$\varphi(t)$ relationship that should hold whenever the tube dilates consistently with the CR mechanism and demonstrated its validity. This result offered an experimental basis for accurate description of the entanglement effect on the motion of multi-branched chains.

Nonlinear Rheology of Multiblock Copolymer Solutions, Matsumiya Y, JAPAN-KOREA Polymer Young Scientist Symposium, Green-pia in Tsunan (Niigata), 24 October 2008 (Invited).

Grants

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

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

Masubuchi Y, New Molecular Model for Branched Polymer Chains, Grant-in-Aid for Scientific Research (B), 1 April 2008–31 March 2010.

Matsumiya Y, Dynamics of Ionic Liquids in Polymer Networks, Grant-in-Aid for Young Scientists (B), 1 April 2007–31 March 2009.

Award

Watanabe H, The Award of the Society of Polymer Science, Japan, "Molecular Dynamics and Rheology of Homogeneous and Inhomogeneous Polymer Liquids", The Society of Polymer Science, Japan, 29 May 2008.

Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

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

Prof
SATO, Naoki
(D Sc)

Assoc Prof
ASAMI, Koji
(D Sc)

Assist Prof
YOSHIDA, Hiroyuki
(D Sc)

Proj Res*
MURDEY, Richard James
(Ph D)

*Assist Prof (SER) of Pioneering Research Unit for Next Generation

Res
KATOH, Keiichi
(D Sc)

Students

KANEKO, Hideo (RF)
HIRAMATSU, Takaaki (D3)
TSUTSUMI, Jun'ya (D3)
FUKUHARA, Sho (M2)
UCHINO, Yosuke (M2)
IMABAYASHI, Hiroki (M1)
KAWAUCHI, Tatsuro (M1)

Scope of Research

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

Research Activities (Year 2008)

Publications

Yoshida H, Sato N: The Crystallographic and Electronic Structures of Three Different Polymorphs of Pentacene, *Phys. Rev. B*, **77**, 235205 (2008).

Asami K: Simulation for the Dielectric Images of Single Biological Cells Obtained using a Scanning Dielectric Microscope, *J. Phys. D: Appl. Phys.*, **41**, 085501 (2008).

Presentations

A Neutral Radical Complex as a "True" Molecular Semiconductor: Lutetium Bisphthalocyanine, Murdey R, Bouvet M, Sato N, 2008 Symposium on Coordination Compounds as Inorganic-Organic Composite Materials (Sanda, Japan), 19 April 2008.

Structures and Electronic Structures of Pentacene Thin Films in Polymorphism, Yoshida H, Sato N, The 14th International Conference on Solid Films and Surface (Dublin, Ireland), 29 June–4 July 2008.

The Evolution of the Energy Band Structure in Polythienoacene; Photoemission Study of Bis(benzo)pentathienoacene as a Function of Film Thickness, Yoshida H, Watazu Y, Sato N, Kawabe E, Yamane H, Kanai K, Seki K, Okamoto T, Yamaguchi S, International Symposium on Molecular Conductors 2008 (Okazaki, Japan), 23–25 July 2008.

Structural Analysis and Energy Band Calculation of Polymorphic Pentacene Thin Films, Yoshida H, Sato N, The 21st IUCr Satellite Meeting "Molecular Crystals Exhibiting Exotic Functions" (Osaka, Japan), 21–22 August 2008.

Single Cell Analysis Using a Scanning Dielectric Microscope, Asami K, The 5th International Conference on Broadband Dielectric Spectroscopy and Its Applications (Lyon, France), 26–29 August 2008.

Grants

Sato N, Development of Novel Electronic Systems Based on Hybridization of Characteristic Molecular Properties and Specific Aggregate Structures, Grant-in-Aid for Scientific Research (2) on Priority Areas of Molecular Conductors, 17 October 2003–31 March 2008.

Asami K, Dielectric Monitoring of Cultured Cells Responding to External Stimuli, Collaboration Research with Sony Corporation (Life Science Laboratory, Material Laboratories), 27 October 2008–31 March 2009.

Yoshida H, The Relation between Electronic Structure and Spin Injection Efficiency at Organic Semiconductor/Metal Interfaces: Towards the Development of Organic Spin Device, Grant-in-Aid for Scientific Research (C), 1 April 2008–31 March 2012.

Correlation between Crystallographic and Electronic Structures of Three Different Polymorphs of Pentacene

The energy bands of three polymorphs of pentacene, i.e., the thin-film, bulk, and single-crystal phases, were calculated. In the calculation of the thin-film phase, we applied the structural data obtained from our recent studies on the X-ray diffraction analysis using the reciprocal space mapping method. The band structures are essentially two-dimensional as shown in Figure 1, i.e., only small dispersions are found along the *c** direction. The energy dispersion of the thin-film phase is examined to be larger and more isotropic than those of the other phases. The energy dispersions of the bands derived from highest occupied molecular orbital (HOMO), HOMO-1, lowest unoccupied molecular orbital (LUMO) and LUMO+1 levels are analyzed by comparing with the corresponding results on the basis of the tight-binding approximation; the dispersions are well described by transfer integrals among only the nearest neighbor molecules. In accordance with this result, a simple model is presented to explain the relation between the crystal structure and the energy dispersion. From the calculated bands, the effective masses are derived to discuss the charge-carrier transport properties in the respective phases. Further, photoemission spectra were measured for the thin-film and bulk phases, to confirm that the observed spectral features of the HOMO-derived bands are interpreted by the calculated density of states.

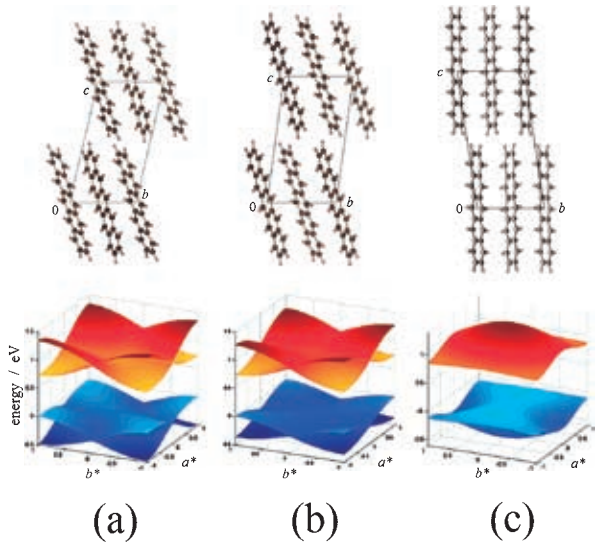


Figure 1. Crystallographic structures and corresponding calculated energy-band structures of pentacene polymorphs: (a) single-crystal phase, (b) bulk phase and (c) thin-film phase.

Dielectric Cytometry of Erythrocytes

Biological cells are polarized in an ac electric field due to charge accumulation at the interfaces between the plasma membrane and the aqueous phases, namely interfacial polarization. The polarization depends on the cell shape as well as the electrical properties of the membrane and the cytoplasm, and therefore the dielectric spectrum of the cell suspension is specific to the cell shape. However, there have been few systematic studies on this issue with erythrocytes, whose shape is susceptible to the metabolic states, the external conditions and diseases. We measured dielectric spectra of four types of erythrocytes as shown in Figure 2 (Hayashi, et al., *Phys. Med. Biol.*, **53**, 2553 (2008)). This figure clearly demonstrates that the spectrum shape or broadening is sensitive to the cell shape and that dielectric spectroscopy is a useful tool for studying the cell shape change. The dielectric spectra of discocytes and echinocytes were respectively simulated with the bicon-cave-discoid model and the spinous-sphere model using the three-dimensional finite difference method (Katsumoto, et al., *Biophys. J.*, **95**, 3043 (2008)). The agreement between the observed and theoretical spectra was satisfactory for both of discocytes and echinocytes. We also devised an efficient method to estimate the capacitance of the plasma membrane and the conductivity of the cytoplasm on the basis of the numerical simulations.

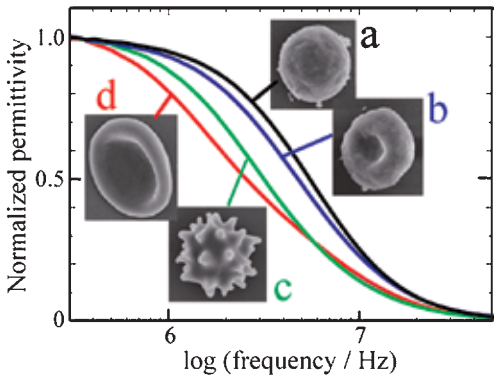


Figure 2. Dielectric spectra of erythrocytes with different shapes. (a) spherocyte, (b) stomatocyte, (c) echinocyte and (d) discocyte.

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Prof
UMEDA, Masato
(D Pharm Sc)

Assoc Prof
IKENOUCHI, Junichi
(D Med Sc)

Assist Prof
KATO, Utako
(D Sc)

Res Associate (pt)

YAMAGUCHI, Yukiko

Students

TANIUCHI, Kentaro (D3)
SUZUKI, Harumitsu (M2)
KUBO, Akira (M2)
GOTO, Mina (M1)

Scope of Research

We have undertaken the molecular biology, cell biology and behavioral genetics approaches to study the role of biological membrane systems in controlling animal morphogenesis and behavior. The membrane is a complex supramolecular complex formed by a noncovalent self-assembly of proteins, lipids, and carbohydrates. Our long term objective is to understand the fundamental principles underlying the dynamism of complex membrane systems and to provide a clue to reconstruct an artificial supramolecular membrane complex. Current research topics are as follows:

(1) Identification of a series of proteins that regulate molecular motion of lipid molecules and elucidation of their role in cellular and animal morphogenesis.

(2) Establishment of a series of *Drosophila* mutants with aberrant temperature preference (*atsugari, samugari*, etc) and elucidation of the molecular relationship between the temperature-responding membrane systems and animal behaviors.

Research Activities (Year 2008)

Publications

Katadae M, Hagiwara K, Wada A, Ito M, Umeda M, Casey PJ, Fukada Y: Interacting Targets of the Farnesyl of Transducin γ-subunit, *Biochemistry*, **47**, 8424-8433 (2008).

Ikenouchi J, Sasaki H, Tsukita S, Furuse M, Tsukita S: Loss of Occludin Affects Tricellular Localization of Tricellulin, *Mollecular Biology of the Cell,* **19**, 4687-4693 (2008).

Shimizu M, Fukunaga Y, Ikenouchi J, Nagafuchi A: Defining the Roles of {beta}-catenin and Plakoglobin in LEF/TCF-dependent Transcription Using {beta}-catenin/plakoglobin-null F9 Cells, *Molecular and Cellular Biology*, **28**, 825-835 (2008).

Presentations

Membrane Phospholipid Flip-flop and Its Role in Cell Motility, Kato U, Inadome H, Umeda M, The 50th Japanese Conference on the Biochemistry of Lipids, 5–6 June 2008, Tokushima.

Transbilayer Movement of Membrane Phospholipids and Its Role in Cell Migration, Kato U, Umeda M, The 60th Annual Meeting of the Japan Society for Cell Biology, 29 June–1 July 2008, Yokohama.

A Role of Delta 9 Fatty Acid Desaturase for Energy Metabolism in *Drosophila melanogaster*, Suzuki H, Kato U, Umeda M, BMB2008, 9–12 December 2008, Kobe.

Grants

Umeda M, Development of Two-dimensional Imaging. Systems of Membrane Lipids Using Intense Femtosecond. Laser Desorption/ionization Mass Spectrometory, Grant-in-Aid for Exploratory Research, 1 April 2006–31 March 2008.

Umeda M, Membrane Lipid Field Produced by Phospholipid Flippase and Its Role in Cytoskeletal Reorganization, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–1 March 2010.

Ikenouchi J, Elucidation of Molecular Mechanisms which Generate and Maintain Discrete Membrane Domains in Polarized Cells, PRESTO, Japan Science and Technology Agency, 1 October 2007–31 March 2011.

Regulation of Membrane Phospholipid Dynamics and Its Role in Cell Migration

The basic structure of biological membranes is the lipid bilayer in which phospholipids distribute asymmetrically between the two leaflets of the bilayer. This asymmetry is regulated by the transbilayer movement of phospholipids, but its physiological significance and molecular mechanisms are largely unknown. Previously we have identified a putative aminophospholipid translocase complex responsible for the inward movement of aminophospholipids, P-type ATPase (ATP8A1) and its non-catalytic subunit mROS3. Depletion of either mROS3 or ATP8A1 inhibited cell migration as well as the inward movement of aminophospholipids across the plasma membrane. ATP8A1 localized at the leading edge of migrating cells and contributes to the formation of membrane ruffles by regulating actin cytoskeleton. Furthermore, PE is exclusively located in the inner leaflet of the plasma membrane at the leading edge (Figure 1). Immobilization of cell-surface PE by a PE-binding peptide inhibited the formation of membrane ruffles, causing a severe defect in cell migration. These results indicate that organized movement of cell-surface PE mediated by ATP8A1 plays an important role in cell migration by regulating actin reorganization and membrane ruffling.

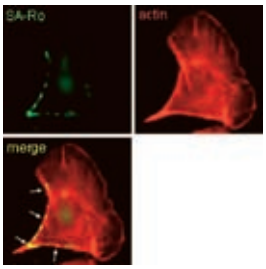

Figure 1. Cell-surface PE distributes in the inner leaflet of the ruffling membranes in migrating cells. The serum-stimulated cells were incubated with 10 μg/ml PE-binding peptide (SA-Ro) for 30 min at 37 ℃, and then fixed and stained for SA-Ro and actin. Arrows indicate the colocalization of SA-Ro and actin at the rear membrane.

Elucidation of Molecular Mechanisms which Generate and Maintain Discrete Membrane Domains in Polarized Cells

The plasma membranes of cells are fundamental components of our body. They are composed of discrete membrane domains in which membrane proteins and lipids are differentially partitioned. Compared to plasma membrane proteins which have been investigated by many researchers, plasma membrane lipids are less well understood, even though they are the other main component of membranes. Using epithelial cells as an experimental model, we aim to clarify what kind of lipids and lipid metabolites are enriched in the apical as well as the basolateral membrane, and how these asymmetric membrane domains are maintained to be separated (Figure 2).

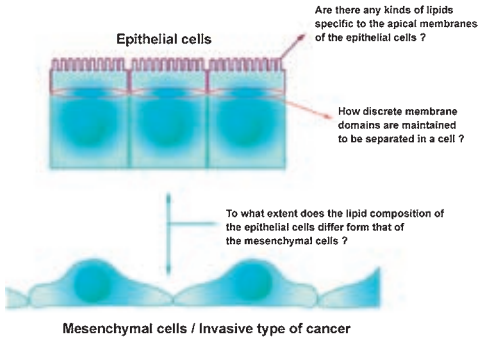

Figure 2.

Drosophila Stearoyl-CoA Desaturase in Energy Metabolism

In many animals, energy-rich components are converted into glycogen and triacylglycerol (TAG), the storage forms of carbohydrate and fat, respectively. TAG is deposited in the adipose tissue in mammals or the fat body in *Drosophila*, and is metabolized during periods of energy need such as nutrient depletion. The regulatory mechanisms of energy homeostasis are still not fully understood. Stearoyl-CoA desaturase, catalyzing introduction of the *cis* double bond in the Δ9 position of fatty acyl-CoA substrates, is a rate-limiting enzyme in the biosynthesis of monounsaturated fatty acids (Figure 3A). We generated a series of *Drosophila* mutants that showed a defective expression of stearoyl-CoA desaturase (desat1). One of them, designated *desat1#42*, showed dramatic reduction in TAG content and was defective in survival during starvation (Figure 3B). In the *desat1#42* mutant, the expression of desat1 was specifically reduced in oenocyte, an organ analogous to mammalian liver. The *desat1#42* mutant will provide a unique model for studying the physiological functions of desat1 in energy metabolism.

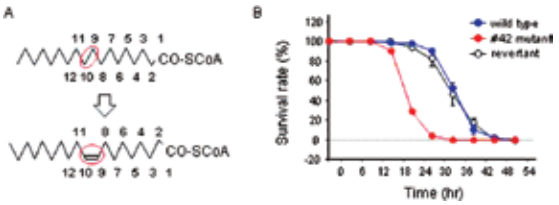

Figure 3. Starvation resistance was reduced in the *desat1#42* mutant flies.
A) Double bond introduction by stearoyl-CoA desaturase
B) Survival rate of wild type and *desat1#42* mutant flies during starvation

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Prof
NODA, Akira
(D Sc)

Assoc Prof
IWASHITA, Yoshihisa
(D Sc)

Assist Prof
SOUDA, Hikaru

Techn
TONGU, Hiromu

Res
FUJISAWA, Hiroshi
(D Sc)

Lecturer (pt)

YAMADA, Satoru (D Sc)
Gunma University Heavy Ion Medical Center

Students

ITOH, Hiroyuki (D3)
ICHIKAWA, Masahiro (D1)
NAKAO, Masao (D1)
SUGIMOTO, Takanori (M2)
YAMADA, Masako (M2)
WAKITA, Akihisa (M2)

Technician(pt)

KAZAMA, Ichiro

Visitors

Dr JAMESON, Robert A — Goethe University, Germany, 8 April–6 June 2008
Dr GRIESER, Manfred — Max Planck Institute, Germany, 17–29 November 2008

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: Compression of the energy spread of laser-produced ion beams by an rf cavity for 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.

Research Activities (Year 2008)

Publications

Wakasugi M, Noda A, Shirai T et al., Novel Internal Target for Electron Scattering off Unstable Nuclei, *Phys. Rev. Lett.*, **100**, 164801 (2008).

Tanabe M, Ishikawa T, Nakao M, Souda H, Ikegami M, Shirai T, Tongu H, Noda A: Longitudinal and Transverse Coupling of the Beam Temperature, *Appl. Phys. Express*, **1**, 028001 (2008).

Fujimoto T *et al.*: Formation and Fast Extraction of a Very Short-bunched Proton Beam for the Investigation of Free Radicals, *Nucl. Instrum. Meth.*, **A588**, 330-335 (2008).

Iwashita Y *et al.*: Variable Permanent Magnet Sextupole Lens for Focusing of Pulsed Cold Neutrons, *Nucl. Instrum. Meth.*, **A586**, 73-76 (2008).

Tajima Y *et al.*: Reduction of Skin Effect RF Power Loss by a Thin Conductor Foil, *Jpn. J. Appl. Phys.*, **47**, 4765-4768 (2008).

Iwashita Y *et al.*: Development of High Resolution Camera for Observations of Superconducting Cavities, *Phys. Rev. ST Accel. Beams*, **11**, 093501 (2008).

Souda H *et al.*: COD Correction for Laser Cooling at S-LSR, *Nucl. Instrum. Meth.*, **A597**, 160-165 (2008).

Presentations

Souda H *et al.*, Alignment of S-LSR, 10th International Workshop on Accelerator Alignment (IWAA08), 12 February 2008, Tsukuba, Japan.

Iwashita Y *et al.*, Development of a High Resolution Camera and Observations of Superconducting Cavities, 11th European Particle Accelerator Conference (EPAC'08), 25 June 2008, Genoa, Italy.

Noda A *et al.*, Present Status of Beam Physics Research using Accelerator Facility of ICR, Kyoto University, The Fifth Annual Meeting of Particle Accelerator Society of Japan/The 33rd Linear Accelerator Meeting, 6 August 2008, Hiroshima, Japan.

Grants

Noda A, Creation of Innovation Centers for Advanced Interdisciplinary Research Areas: Photo-Medical Valley,

Laser Cooling of a Mg^+ Ion Beam at S-LSR

Laser cooling experiments of $^{24}Mg^+$ ion beams with the kinetic energy of 40 keV have been carried out at an ion storage and cooler ring, S-LSR. A transition between $3s^2S_{1/2}$-$3p^2P_{3/2}$, corresponding to a laser wavelength of 280nm at laboratory frame is utilized. A laser with this wavelength is attained by a frequency doubler applied to the output from a ring dye laser pumped by a Nd:YVO_4 laser.

Figure 1 shows the dependence on the cooled ion number of the equilibrium longitudinal temperature realized by the beam cooling with the use of a co-propagating laser and an induction deceleration [1]. With cooling, the relation between particle numbers N and longitudinal temperatures $T_{\|}$ is measured as $T_{\|} = 0.14N^{0.32}$. The attained lowest longitudinal temperature, 3.6 K, is limited by higher temperature of transverse directions, which are weakly coupled with that of longitudinal direction by an intra beam scattering.

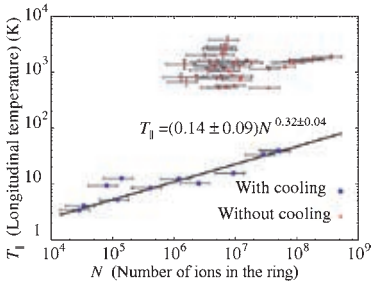

Figure 1. Equilibrium longitudinal temperature of the beam cooling for various numbers of circulating ions.

According to this result, it is necessary to reduce temperature for further cooling. Theoretically, transverse laser cooling is to be achieved by coupling of longitudinal and transverse degrees of freedom by synchro-betatron resonance. In Figure 2, momentum spreads after application of the longitudinal beam cooling for the bunched beam with various synchrotron tunes are shown. In this figure, sharp peaks of momentum spreads appear for the conditions where synchrotron tune and horizontal betatron tune, ν_s and ν_x, are 0.064 and 2.065 or 0.057 and 2.054. This result means longitudinal cooling rates are reduced when the resonance condition is satisfied. It is considered as an indication of longitudinal and transverse coupling. Further experiments to demonstrate transverse cooling by observing the transverse size reduction associated to a longitudinal beam cooling is now under preparation.

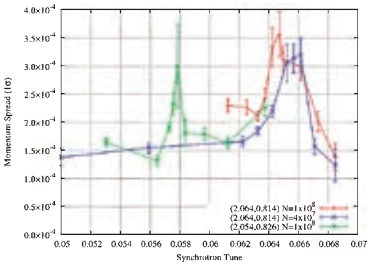

Figure 2. Momentum spreads of laser-cooled bunched ion beams for various synchrotron tunes.

Proof of Principle Experiment of Electron Nucleus Scattering with use of SCRIT (Self-Confining Radioactive Isotope Ion Target) installed into KSR

With the use of an electron storage ring, KSR, the studies of the structure of nucleus trapped into an ion trap: SCRIT (Self-Confining Radioactive Isotope Ion Target) set in a straight section of KSR as shown in Figure. 3 has been performed in these a few years by collaboration with a group from RIKEN. Recently the principle of such a scheme to investigate the structure of the nucleus detecting the scattered particles by an electron-nucleus scattering has been successfully demonstrated for stable ions as ^{133}Cs, although the final aim of such a scheme is to be applied for unstable nuclei [2].

Figure 3. An overall view of an electron storage ring, KSR, where the SCRIT is installed.

[1] Tanabe M *et al.*, *Appl. Phys. Express* **1**, 028001 (2008).
[2] Wakasugi M *et al.*, *Phys. Rev. Lett.* **100**, 164801 (2008).

Special Coordination Funds for Promoting Science and Technology, 1 June 2007–31 March 2010.

Iwashita Y, Application and Development of Super Strong Permanent Magnet Especially for Linear Collider and Neutron Optics, Grant-in-Aid for Scientific Research, (A) (1), 1 April 2006–31 March 2009.

Iwashita Y, Development of Satellite Compact Pulse Neutron Source, Joint Development Research at High Energy Accelerator Research Organization (KEK), 1 April 2007–31 March 2008.

Souda H, Three-dimensional Crystalline Beam by Laser Cooling and Beam Orbit Control, Grant-in-Aid for Scientific Research for JSPS Fellow, 1 April 2007–31 March 2009.

Award

Yamada M, Poster Prize, Development of the Permanent Magnet Sextupole Lens for Focusing of Pulsed Neutron Beam, 8th Annual Meeting of the Japanese Society for Neutron Science, 2 December 2008.

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

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

Prof
SAKABE, Shuji
(D Eng)

Assoc Prof
HASHIDA, Masaki
(D Eng)

Assist Prof
TOKITA, Shigeki
(D Eng)

Proj Res
OHTANI, Kazuto
(D Sc)

Students

MASUNO, Shinichiro (D2)
NAMBA, Shin (M2)
INOUE, Shunsuke (M1)
OKAMURO, Kiminori (M1)
HIROKANE, Mayu (M1)
JAHANGIRI, Fazel (RS)

Visitors

Dr KOFLER, Heinrich — Vienna University of Technology, 2 February 2008
Prof SHIMIZU, Hirohiko — High Energy Accelerator Research Organization, 10 October 2008

Scope of Research

Recent remarkable progress of ultra-intense ultra-shot lasers has opened the new field of intense laser science. 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, x-ray, ions, THz, and so on), which have the features of point, pulse, intense, compact, and perfect synchronized sources with different radiations. The radiations 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 of soft matter, molecules, nano-scale matter, and so on is also the next-generation laser processing. In our laboratory ultra intense femtosecond laser named T^6-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

Research Activities (Year 2008)

Publications

Hashida M, Sakabe S: Carbon Nanotubes Cathode Modified by Femtosecond Laser Ablation, *O pluse E*, **30**, 461-464 (2008) (in Japanese).

Tokita S, Hashida M, Masuno S, Namba S, Sakabe S: 0.3% Energy Stability, 100-Millijoule-Class, Ti:Sapphire Chirped-Pulse Eight-Pass Amplification System, *Optics Express*, **16**, 14875-14881 (2008).

Presentations

Femtosecond Laser Ablation of Carbon Nanotubes Cathode, Hashida M, Shimizu S, Sakabe S, 28th Annual Meeting of The Laser Society of Japan, Nagoya, 30 January 2008 (invited).

Sapphire-Conductive End-Cooling of High Power Cryogenic Yb:YAG Lasers, Tokita S, Kawanaka J, Fujita M, Kawashima T, Izawa Y, 28th Annual Meeting of The Laser Society of Japan, Nagoya, 31 January 2008 (invited).

Basic of Ultrashort Pulse Laser Material Processing, Hashida M, Laser Expo 2008, Yokohama, 25 April 2008 (invited).

Self-Organization of Periodic Grating Structure on Metal Surface by Femtosecond Laser Pulses, Sakabe S, Hashida M, Tokita S, Namba D, Okamuro K, 4th Asian Symposium on Intense Laser Science 2008, Gwangju, Korea, 5 November 2008 (invited).

Application of Femtosecond Laser Material Processing, Hashida M, The 11th Optical Science Seminar, Miyazaki, 21 November 2008 (invited).

Grants

Sakabe S, et al., Time Resolved Electron Microscope with Intense Femtosecond Laser Produced Electrons, Grant-in-Aid for Scientific Research (A), 1 April 2006–31 March 2010.

Femtosecond Laser Nano-ablation of Metal

Nano-ablation of copper has been demonstrated with an intense femtosecond laser. In order to investigate the mechanism of nano-ablation of metal, the emitted ions were measured by a time-of-flight mass spectrometer. For ion measurement the laser was irradiated with an incidence angle of 60° relative to the surface normal. The distance from the cupper sample to a MCP ion detector was 1.45 m and the pressure was maintained to ~3×10^{-7} Pa. By laser matter interactions, high-energy Cu^{+} ions are emitted, which cannot be produced by thermal ablation of metal. The ion energy shows contribution of ion Coulomb explosion rather than that of thermal expansion to generate high energy ions.

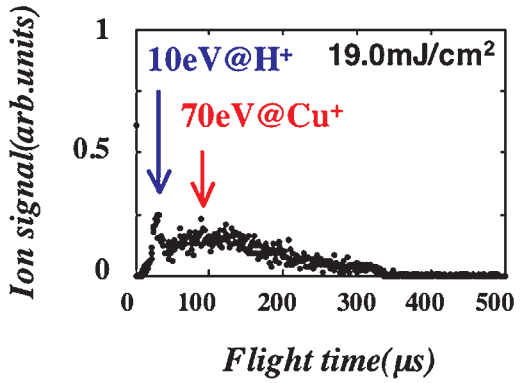

Figure 1. TOF spectrum of copper ablated by femtosecond laser (λ = 800 nm, τ = 130 fs, F = 19 mJ/cm^2, s-polarization).

A Novel Method for Ultrafast Time -Resolved Electron Diffraction

Observation of atomic motions on ultrafast time scales (less than 1 ps) is a very attractive approach to acquire new knowledge about the evolution of new phases in solids, the kinetic pathways of chemical reactions, and the biological functioning processes. The ultrafast electron diffraction (UED) with electrons field-emitted from a photocathode is a very promising method for the direct observation of non-equilibrium chemical structures at the atomic-level space and femtosecond time scales. This method, however, has an inevitable problem of broadening of the electron-pulse duration due to space-charge (Coulomb repulsion) effects. On the ground of this pulse broadening, the temporal resolution of the UED method is easily and seriously reduced when the number of electrons per pulse increases. Some proposals and experiments to overcome this problem have been recently introduced, but are not yet demonstrated or have significant defects. Our idea to solve this problem is to use laser acceleration of electrons in plasma. The laser acceleration provides an extremely strong acceleration field in plasma compared with electro-static or RF accelerations. This allows the space-charge effects to be minimized. We have started the development of this novel UED method and succeeded in the demonstration of getting the picture of electron diffraction patterns using the laser accelerated electron pulses (Figure 2). This achievement strongly indicates the high feasibility of the new present method.

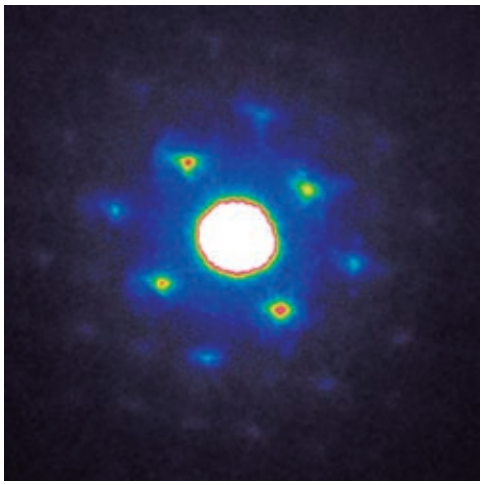

Figure 2. Electron diffraction pattern of a gold single crystal obtained using the laser accelerated electron pulses.

Hashida M, Advanced Material Processing with Femtosecond Lasers, Iketani Science and Technology Foundation, 20 July 2007–31 March 2008.

Hashida M, Improvement of Ablation Rate for Femtosecond Laser Processing, Amada Foundation for Metal Work Technology, 20 December 2007–31 March 2009.

Hashida M, Study on Mechanism of Metal Ablation by Short Pulse Laser, The Murata Science Foundation, 25 July 2008–31 March 2009.

Tokita S, Development of Mid-Infrared High-Power Ultrashort-Pulse Fiber Laser, Grant-in-Aid for Young Scientists (B), 1 April 2008–31 March 2010.

Tokita S, Development of Ultrafast Time-Resolved Electron Diffraction Method for Dynamic Structure Analysis in Femtosecond Time Scale, Iketani Science and Technology Foundation, 1 April 2008–31 March 2009.

Tokita S, Development of Mid-Infrared Femtosecond Fiber Laser using Fluoride Grass Fibers, Amada Foundation for Metal Work Technology, 15 December 2008–31 March 2010.

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

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Prof
ISODA, Seiji
(D Sc)

Assoc Prof
KURATA, Hiroki
(D Sc)

Assist Prof
OGAWA, Tetsuya
(D Sc)

Assist Prof
NEMOTO, Takashi
(D Sc)

Res Associate
MORIGUCHI, Sakumi
(D Sc)

Proj Res
YOSHIDA, Kaname
(D Sc)

Researcher

HATSU, Takako

Guest Scholar

CHOMSAENG, Natthaphol

Students

KIYOMURA, Tsutomu (D3)
HARUTA, Mitsutaka (D2)
SHINODA, Yasuhiro (M2)
UMEDA, Azumi (M2)
OMORI, Yuuki (M1)

Visitors

Prof WU, Maw-Kuen	Academia Sinica, Taiwan, 13–16 March 2008
Prof CHOU, Li-Jen	National Tsing-Hua University, Taiwan, 23–25 March 2008
Prof YAN, Shouke	Chinese Academy of Sciences, China, 16 May 2008
Prof LIU, Tianxi	Fudan University, China, 21 May 2008
Prof GAO, Min	Peking University, China, 21 May 2008
Prof KIRKLAND, Angus	University of Oxford, UK, 28 May 2008

Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. It aims to explore new methods for imaging and also obtaining chemical information in thin films, nano-clusters, interfaces, and even in solutions. 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.

Research Activities (Year 2008)

Publications

Kurata H, Isoda S, Tomita K (JEOL): Development of Nanotip Field Emission Gun, *Kenbikyou*, **42**, 211-213 (2007) (*in Japanese*).

Haruta M, Yoshida K, Kurata H, Isoda S: Atomic Resolution ADF-STEM Imaging of Organic Molecular Crystal of Haloganated-Cu-phthalocyanine, *Ultramicroscopy*, **108**, 545-551 (2008).

Yoshida K, Jiu J (Osaka Univ.), Nagamatsu D, Nemoto T, Kurata H, Adachi M (Doshisha Univ.), Isoda S: Structure of TiO_2 Nanorods Formed with Double Surfactants, *Mol. Cryst. Liq. Cryst.*, **491**, 14-20 (2008).

Grants

Kurata H, Development of an EELS/XES Electron Microscope for Electronic Structure Analysis, Leading Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004–31 March 2007.

Kurata H, Local State Analysis of Defects and Interface Regions by Spherical Aberration Corrected STEM and

Local State Analysis by STEM-EELS Equipped with a Nanotip-FEG

Electron energy-loss spectroscopy (EELS) combined with an aberration corrected scanning transmission electron microscope (STEM) enable to perform local analysis with an atomic resolution owing to a sub-angstrom electron probe with a high probe current. In order to enhance a performance of STEM-EELS analysis, we developed a 200 kV Cs-corrected STEM/TEM equipped with a nanotip-FEG, which produces an incident electron probe of 0.1 nm or less in diameter with an illumination semi-angle of 23 mrad. As an application to STEM-EELS analysis, we carried out local state analysis using the spatially resolved EELS measured from a $BaTiO_3$ (BTO) thin film grown on $SrTiO_3$ (STO) substrate. In the vicinity of the interface, a strained structure and a misfit dislocation are observed in the BTO region. The imaginary part of dielectric function (ε_2 spectrum) deduced from valence electron excitation spectrum shows the change of electronic structure due to the strain structure near the interface, which is confirmed by a first principles band structure calculation. From the energy-loss near-edge structure of Ti $L_{2,3}$-edge, the crystal-field strength measured from the separation between t_{2g} and e_g peaks is also slightly different, which indicates that the local electronic structure should be changed at the strained and defect regions.

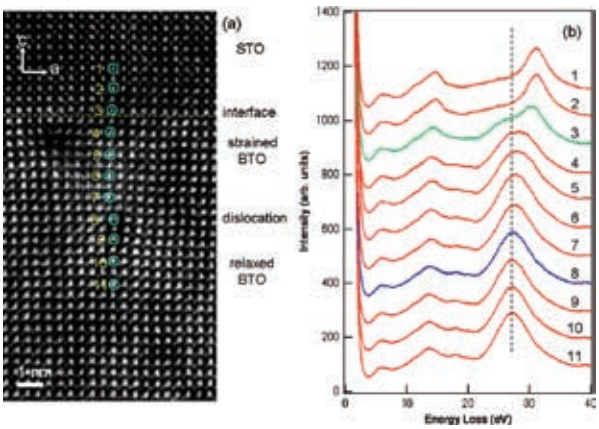


Figure 1. STEM image and spatially resolved EELS measured from the vicinity of the interface of BTO/STO.

Atomic Resolution ADF-STEM Imaging of Organic Molecular Crystal of Haloganated-Cu-phthalocyanine

Annular dark-field (ADF) scanning transmission electron microscopy (STEM) is a powerful technique for acquiring high-resolution images of materials. High-angle ADF (HAADF) STEM images are considered to be incoherent, showing chemical image contrast (Z-contrast), due to the dominated effect of thermal diffuse scattering (TDS) in the detected signal. However, to date, HAADF STEM imaging has been performed invariably for inorganic crystals. In this report, an ADF-STEM measurement is demonstrated for the first time to be applicable for acquiring Z-contrast images of organic molecules at atomic resolution. The structural image of a molecular crystal of hexadecachloro-Cu-phthalocyanine (Cl_{16}-CuPc) is acquired at atomic resolution by ADF-STEM (Figure 2). In molecular crystals with comparatively large lattice constants, such as the Cl_{16}-CuPc sample examined in this study, low-angle ADF (LAADF) STEM observation with a detection angle of 24–64 mrad was found to be advantageous for acquiring incoherent Z-contrast images similar to the case of conventional HAADF-STEM.

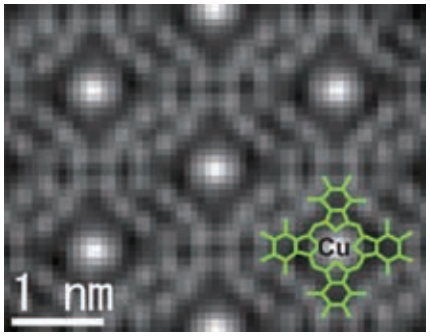


Figure 2. Noise filtered LAADF-STEM image of Cl_{16}-CuPc projected along the c-axis.

EELS, Grant-in-Aid for Scientific Research (B)19310071, 1 April 2007–31 March 2010.

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2007–31 March 2011.

Isoda S, Development of Observation Method of Polymer Composite Materials without Staining by Scanning Transmission Electron Microscope, Grant-in-Aid for Scientific Research (C) 20550188, 1 April 2008–31 March 2011.

Award

Koshino M, Kurata H, Isoda S, Microscopy and Microanalysis, 2007 Best Materials Paper Award, "Stability Due to Peripheral Halogenation in Phthalocyanine Complexes", Microscopy Society of America, 10 September 2008.

Advanced Research Center for Beam Science
- Structural Molecular Biology -

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

Prof
HATA, Yasuo
(D Sc)

Assoc Prof
ITO, Yoshiaki
(D Sc)

Assist Prof
FUJII, Tomomi
(D Sc)

Proj Res*
YAMAUCHI, Takae

*Assist Prof of Institute of Sustainability Science

Res
TOCHIO, Tatsunori
(D Sc)

Res
HANDA, Katsumi
(D Sc)

Students

ATSUTA, Hideki (M2)
UCHIDA, Kenji (M1)
KOBAYASHI, Kazutaka (M1)

Scope of Research

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

Research Activities (Year 2008)

Publications

Fujii T, Goda Y, Yoshida M, Oikawa T, Hata Y: Crystallization and Preliminary X-ray Diffractrion Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Cryst.*, **F64**, 737-739 (2008).

Fujii T, Oikawa T, Muraoka I, Soda K, Hata Y: Crystal Structure of Tetrameric Malate Dehydrogenase from Antarctic Psychrophile, *Acta Cryst.*, **A64**, C255-256 (2008).

Presentation

Crystal Structure of Tetrameric Malate Dehydrogenase from Antarctic Psychrophile, Fujii T, Oikawa T, Muraoka I, Soda K, Hata Y, XXI Congress and General Assembly of the International Union of Crystallography, 29 August 2008, Osaka, Japan.

X-Ray Diffraction Studies of GraC Involved in Resorcinol Catabolim of *Rhizobium*

Rhizobium is a genus of tubercle-forming bacteria. It grows in the root of a plant in symbiosis with other bacteria to fix nitrogen from the air. Although much attention has been paid to the *Rhizobium* genes and gene products, there is still little information available on the molecular structure, function, and detailed properties of the enzymes involved in its metabolic pathways. In the course of a screening experiment, *Rhizobium* sp. strain MTP-10005 was isolated from natural river water. Enzymological studies showed that the *graD*, *graA*, *graB*, and *graC* genes of the bacterium encode the reductase (GraD) and oxidase (GraA) components of resorcinol hydroxylase, hydroxyquinol 1,2-dioxygenase (GraB), and maleylacetate reductase (GraC), respectively. In order to reveal their structures and functions, we have been performing X-ray structural studies of the enzymes.

Maleylacetate reductase (GraC) from *Rhizobium* sp. strain MTP-10005 catalyzes NADH- or NADPH-dependent reduction of maleylacetate to 3-oxoadipate. The polypeptide chain of the enzyme consists of 351 amino acid residues. The amino-acid sequence of the enzyme is homologous to those of maleylacetate reductases from *Ralstonia eutropha* JMP134, *Pseudomonas* sp. strain B13, and *Agrobacterium tumefaciens*. These homologous enzymes are known to be inhibited by thiol-blocking reagents such as *p*-chloromercuribenzoate and Hg^{2+}. The sequence homology suggests that this inhibition might be conserved in the present enzyme GraC.

Initial crystallization experiments were performed by the hanging-drop vapour-diffusion method using Crystal Screens I and II (CS I, II). The final conditions based on those of CS II#32 produced rhombohedron-shaped crystals with approximate dimensions of 0.30 × 0.20 × 0.05 mm at 293 K in 3 d using the sitting-drop vapour-diffusion method (Figure 1). Drops of 1 μl protein solution at 8 mg ml^{-1} (in 50 mM Tris-HCl buffer, pH 8.0) and 1 μl reservoir solution were equilibrated against 500 μl reservoir solution consisting of 1.4 M ammonium sulfate, 0.1 M sodium chloride, 2% (w/v) benzamidine HCl, and 0.1 M NaHEPES, pH 7.5. The drops were microseeded using the original crystals grown in CS II#32.

Figure 1. Crystal of maleylacetate reductase (GraC) from *Rhizobium* sp. strain MTP-10005. The dimensions of the crystal were approximately 0.30 × 0.20 × 0.05 mm.

Diffraction experiments were performed at beamline BL6A, Photon Factory, Tsukuba, Japan. The native crystal with typical dimensions 0.25 × 0.20 × 0.05 mm was soaked into a cryoprotectant solution consisting of 1.4 M ammonium sulfate and 25% (v/v) glycerol for less than ten seconds, and flash-cooled in a nitrogen stream at 100 K. Diffraction data were collected at a wavelength of 1.000 Å using a Quantum 210 CCD detector set to 166.2 mm in a crystal-to-detector distance. The data set was collected at 1.96 Å resolution and has 44,689 independent reflections with completeness of 99.5%.

To solve the phase problem, one kind of heavy-atom isomorphous derivative crystal was prepared by soaking the native crystal in the reservoir solution containing 0.025 mM ethylmercury thiosalicylate (EMTS) for 20 hours. Then, the multi-wavelength anomalous diffraction (MAD) method was applied for solution of the phase problem. Before data collection, XAFS experiments were carried out with this derivative crystal. The absorption spectrum obtained from this experiment was used to fix the wavelengths at four sites (Peak, Edge, Remote-H and Remote-L) around the X-ray absorption L-edge of Hg^{2+} (Figure 2). Besides, the spectrum was analyzed to determine the dispersion and absorption components (f' and f") of Hg^{2+} for the anomalous dispersion correction at their wavelengths (Table 1).

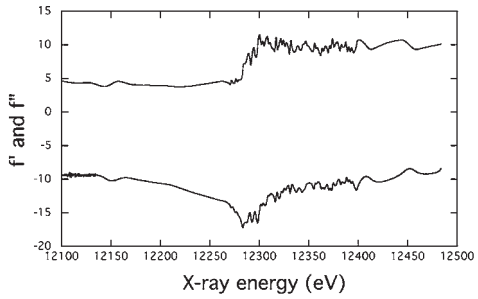


Figure 2. Anomalous scattering factors near the absorption L-edge of mercury from a derivative crystal.

Table 1. Wavelengths and anomalous scattering factors obtained from XAFS experiments

	Peak	Edge	Remote-H	Remote-L
Wavelength (Å)	1.00798	1.00940	0.99923	1.01352
f'	–14.56	–17.22	–8.54	–11.99
f"	11.49	6.50	10.09	3.92

The MAD data sets were collected at 3 Å resolution for the same derivative crystal by irradiation of X-rays with the above four wavelengths. Each of four data sets has about 12,800 independent reflections with completeness of over 99.5%. The structure analysis of GraC is underway in calculating phase angles and electron densities.

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

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

Prof
NAKAMURA, Masaharu
(D Sc)

Assoc Prof
TAKAYA, Hikaru
(D Eng)

Assist Prof
HATAKEYAMA, Takuji
(D Sc)

PD
SEIKE, Hirofumi
(Ph D)

PD (JSPS)
ISHIZUKA, Kentaro
(D Sc)

Students

ITO, Takuma (D2)
YOSHIMOTO, Yuya (D2)
HASHIMOTO, Toru (D1)
KAWAMURA, Shintaro (M2)
FUJIWARA, Yuichi (M2)
NAKAGAWA, Naohisa (M2)
HASHIMOTO, Sigma (M1)
FUKUI, Sadayuki (M1)
YOSHIDA, Kyohei (M1)
SASANO, Daisuke (UG)
ZENMYO, Takeshi (UG)

Visitors

Prof KÜNDIG, E Peter	University of Genova, Switzerland, 29 May 2008
Prof KOTORA, Martin	Charles University, Czech Republic, 14 July–14 October 2008
Dr YAMADA, Yoichi M. A.	RIKEN, Japan, 6 November 2008
Prof SUZUKI, Akira	Hokkaido University, Japan, 21 November 2008
Prof YAMANAKA, Masahiro	Rikkyo University, Japan, 21 November 2008
Prof MOROKUMA, Keiji	Fukui Memorial Research Institute, Kyoto University, Japan, 9 December 2008

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) 3d-transition metal catalyzed controlled Carbon–Carbon bond forming reactions which exploit universal metals such as iron, magnesium and aluminum (2) development of smart materials based on synergistic effect of various metals on peptide (3) understanding and design of synergistic effects of multi-element center interactions for the catalysis with the help of quantum chemical methods and spectroscopy.

Research Activities (Year 2008)

Publications

Fujimoto T, Endo K, Tsuji H, Nakamura M, Nakamura E: Construction of Chiral Quaternary Carbon Center by Indium-Catalyzed Asymmetric α-Alkenylation of β-Ketoesters, *J. Am. Chem. Soc.*, **130**, 4492-4496 (2008).

Hatakeyama T, Nakamura M, Nakamura E: Diastereoselective Addition of Zincated Hydrazones to Alkenylboronates and Stereospecific Trapping of Boron/Zinc Bimetallic Intermediates by Carbon Electrophiles *J. Am. Chem. Soc.*, **130**, 15688-15701 (2008).

Hatakeyama T, Yoshimoto Y, Toma G, Nakamura M: Iron-Catalyzed Enyne Cross-Coupling Reaction, *Org. Lett.*, **10**, 5341-5344 (2008).

Hatakeyama T, Kondo Y, Fujiwara Y, Takaya H, Ito S, Nakamura E, Nakamura M: Iron-Catalysed Fluoroaromatic Coupling Reactions under Catalytic Modulation with 1, 2-Bis(diphenylphosphino)benzene, *Chem. Commun*. in press.

Presentations

Controlling the Iron Catalysis in Cross-Coupling and Some Related Reactions, Nakamura M, The 9th Youngnam-Kinki Joint Symposium on Organometallic Chemistry, Katsura, Kyoto, 24 January 2008.

Controlling Iron-Catalysis in Selective Carbon-Carbon Bond Formations, Nakamura M, The 3rd International

Enyne Cross-Coupling

Transition metal-catalyzed cross-coupling reactions are one of the most powerful tools in organic synthesis. Palladium and nickel catalysts have been the dominant choice for such a purpose, and are widely used in academia as well as in industry. Whereas iron, a practically ideal transition metal, has been actively investigated as a catalyst in the field of cross-coupling reactions, enyne cross-coupling has remained a challenge because of considerable stability and poor reactivity of alkynyl iron intermediate. We have developed efficient enyne cross-coupling of alkenyl halides and triflates with alkynyl magnesium reagents using lithium bromide as a crucial additive, which would accelerate reductive elimination from alkynyl iron intermediate.

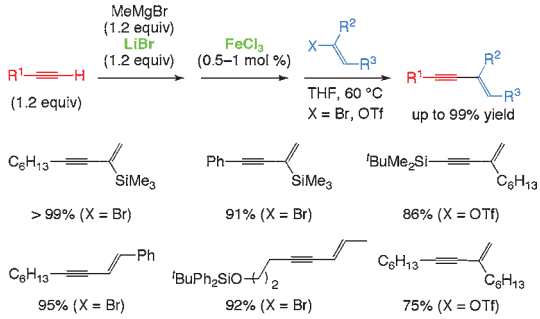


Figure 1. Enyne cross-coupling.

Cross-Coupling of Alkyl Halides with Alkenylzinc Reagents

Cross-coupling reaction of carbon electrophiles with alkenylmetal reagents is a useful method for olefin synthesis. During the past decade, the scope of the alkenyl coupling has been extended by developing efficient cross-coupling of alkyl halides with alkenylmetal reagents by using copper, palladium, cobalt and iron catalysts. There have been, however, considerable limitations to be solved (e.g. insufficient yields from secondary alkyl halides, nonavailability of alkyl chlorides). We have developed a powerful protocol for alkyl-alkenyl coulping, which has been accomplished by combination of readily available alkenylzinc reagents, iron precatalyst, and TMEDA as an additive. This reaction has several synthetically attractive features: (1) high-yielding, (2) chemoselective, (3) stereospecific, and shows broader substrate scope.

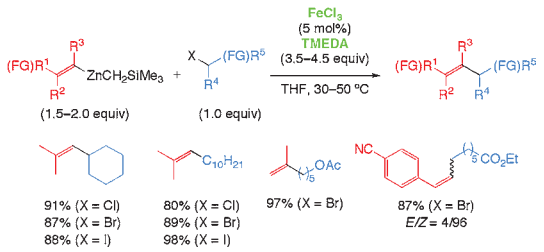


Figure 2. Cross-coupling of alkyl halides with alkenylzinc reagents.

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

The focus of this project is to research the following challenges: i) Development of fundamental method to create composition- and configuration-controlled heterometallic hybrid molecules using metallated-amino acids and peptides as metal units. Programmable metal unit arrangement through chemical synthesis and self-assembly process is employed in complementary to control the composition, 1D/2D array, and 3D configuration of metals on peptides. ii) Screening the function of heterometallic hybrid molecules. Application to supramolecular gelators, molecular electronic devices, photochemical devices, advanced catalysts, artificial enzymes, and MRI contrast agents will be explored with a diverse library of metallated-amino acids and peptides.

Conference on Cutting-Edge Organic Chemistry in Asia under Asian Core Program (ICCEOA-3), Hangzhou, China, 19–23 October 2008.

Grants

Nakamura M, Development of New Synthetic Organic Reactions Based on the Universal Metals Catalysis, Grant-in-Aid for Young Scientists (S), 1 April 2008–31 March 2013.

Nakamura M, Design of Transition Metal/Main Group Elements Synergetic Reagent and Its Synthetic Application, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2010.

Takaya H, A New Approach to Chemical Atom Manipulation: Programmable Metal Unit Arrangement on Peptides to Create Composition- and Configration-Controlled Heterometallic Hybrid Materials, Precursory Research for Embryonic Science and Technology, 1 April 2006–31 March 2010.

Hatakeyama T, Cross-Coupling Reaction Controlled by Fluoride Ion and Carbene Ligand, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Award

Takaya H, The Presentation Award for Young Chemists, The 88th Annual Meeting of the Chemical Society Japan, "Programmable Metal Unit Arrangement on Peptides to Create Combination and Configuration-Controlled Organometallic Materials", Tokyo, 29 March 2008.

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

http://msk2.kuicr.kyoto-u.ac.jp/~shimak-lab/indexE.html

Prof
SHIMAKAWA, Yuichi
(D Sc)

Assoc Prof
AZUMA, Masaki
(D Sc)

Assist Prof
SAITO, Takashi
(D Sc)

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

PD
LONG, Youwen
(D Sc)

PD
TENG, Yonghong
(D Eng)

Post-Doctoral Research Fellow

SMIRNOVA, Olga (D Sc)

Students

NISHIMURA, Kousuke (D3)
KAWAI, Masanori (D2)
OKA, Kengo (D2)
NAKAMURA, Yoshitaka (D1)
HORIKAWA, Takenori (M2)
INOUE, Satoru (M2)
TOYAMA, Takenori (M1)
MATSUMOTO, Kazuya (M1)

Visitors

IWANOWSKA, Monika	University of Rennes 1, France, 16 February–21 July 2008
GRANDSIRE, Anne-Flore	University of Montpellier, France, 20 June–20 August 2008
Prof PAULUS, Werner	University of Rennes 1, France, 1 April 2008
Prof YUSUF, S, M	Bhabha Atomic Research Centre, India, 13 June 2008
Dr ARGYRIOU, Dimitri	Helmholtz Zentrum Berlin, Germany, 22 August 2008
Dr dos SANTOS, Antonio Moreira	Oak Ridge National Laboratry, USA, 22 August 2008
Prof WOODWARD, Patrick M	Ohio State University, USA, 27 August 2008
Prof CHOU, Fang-Cheng	National Taiwan University, Taiwan, 1–5 September 2008

Scope of Research

Transition-metal oxides show lots of interesting and useful properties. They include ferroelectrics, ferromagnets, conductors, batteries, and so on. These materials are widely used in current electronic devices. The wide variety of their crystal structures gives rise to various electronic structures, which lead to interesting and useful physical and chemical properties. We are focusing on the fundamental physics and chemistry of these “functional oxides” and seeking new materials with new functions. We are conducting systematic studies of material synthesis based on phase equilibrium information. Precise crystal structures are analyzed by X-ray and neutron diffractions. Electronic and magnetic structures are discussed based on the results of electronic structure calculations and physical property measurements.

Research Activities (Year 2008)

Publications

Yamada I, Takata K, Hayashi N, Shinohara S, Azuma M, Mori S, Muranaka S, Shimakawa Y, Takano M: A Perovskite Containing Quadrivalent Iron as a Charge-disproportionated Ferrimagnet, *Angew. Chem. Int. Ed.*, **47**, 7032-7035 (2008).

Shimakawa Y: A-site Ordered Perovskites with Intriguing Physical Properties, *Inorg. Chem. Mat. Forum*, **47**, 8562-8570 (2008).

Oka K, Yamada I, Azuma M, Sato K, Takeshita S, Koda A, Kadono R, Takano M, Shimakawa Y: Magnetic Ground State of Perovskite $PbVO_3$ with Large Tetragonal Distortion, *Inorg. Chem.*, **47**, 7355-7359 (2008).

Inoue S, Kawai M, Shimakawa Y, Mizumaki M, Kawamura N, Watanabe T, Tsujimoto Y, Kageyama H, Yoshimura K: Single-crystal Epitaxial Thin Films of $SrFeO_2$ with FeO_2 "infinite layers", *App. Phys. Lett.*, **92**, [161911-1]-[161911-3] (2008).

Single-crystal Thin Films of Infinite-layer Structure $SrFeO_2$ with Square-planer Coordination of Fe^{2+} Ions

There are a number of oxides with transition-metal ions such as Fe, Co, and Ni. Ionic states of the transition metals can vary in the oxides. For strontium (Sr) and iron (Fe) containing perovskite-structure oxides, the oxygen content and Fe ionic state were considered to change between $SrFeO_3$ and $SrFeO_{2.5}$. Last year a new compound, infinite-layer structure $SrFeO_2$, was reported in Nature to be synthesized by using a low temperature reduction with CaH_2.

Immediately after this report, we succeeded in preparing "single-crystal thin films of infinite-layer structure $SrFeO_2$". A $SrFeO_{2.5}$ precursor thin film was first deposited by a pulsed-laser-deposition method and the film was then reduced at low temperature with CaH_2. The resultant sample was confirmed to be a single-crystal infinite layer $SrFeO_2$ from X-ray diffraction and absorption experiments.

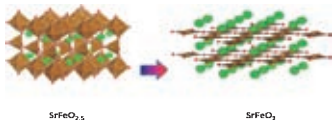


Figure 1. Crystal Structure of $SrFeO_{2.5}$ and $SrFeO_2$.

With the epitaxially grown thin-film samples, we can investigate mobile behaviors of oxygen ions. The results on high oxygen mobility will be useful for fuel-cell applications. The study on single-crystal thin-film samples will also reveal anisotropic crystal and electronic structures of the compound. New physical properties of the infinite-layer structure may appear by using epitaxial strain from the substrate lattice. The present success of preparing the single-crystal thin film $SrFeO_2$ has great impacts on not only research fields of fundamental solid state physic and chemistry but also application fields of new material synthesis with new functions.

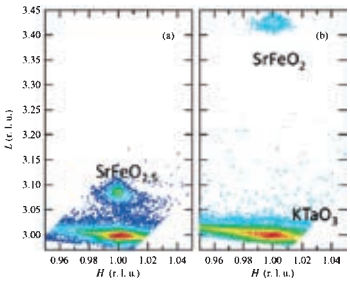


Figure 2. X-ray diffraction of $SrFeO_{2.5}$ and $SrFeO_2$.

$PbTiO_3$ and $BiCoO_3$ with Large Polar Distortions

$PbTiO_3$-based ferroelectric and piezoelectric materials are widely used in memory devices, actuators, and transducers. The search for new ferroelectric and piezoelectric perovskites had been limited to the systems with d^0 ions such as Ti^{4+}, Nb^{5+}, and Ta^{5+} in the B-sites of a perovskite ABO_3. We have investigated perovskites stabilized at high pressures with other transition metals in the B-site and lead or bismuth in the A-site. As results, $PbVO_3$ and $BiCoO_3$ are found to be isostructural with $PbTiO_3$. These have tetragonal distortions (c/a = 1.229 for $PbVO_3$ and 1.267 for $BiCoO_3$) much larger than that of $PbTiO_3$ (c/a = 1.062). The magnetic properties of $PbVO_3$ were the key to understand the origin of this large polar distortion. The temperature dependence of the measured magnetization of multidomain single-crystal samples showed a broad maximum centered around 180 K, indicating a two-dimensional antiferromagnetism with frustration. The two-dimensional magnetism is due to the ordering of d_{xy} orbitals, which is thought to also be related to the large tetragonal distortion of $PbVO_3$.

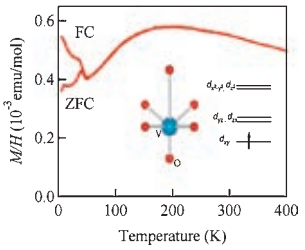


Figure 3. Temperature dependence of magnetic susceptibility of $PbVO_3$ crystal and a schematic drawing of orbital ordering due to a large tetragonal distortion.

Presentations

Complex Ordered Perovskites with Intriguing Physical Properties: Shimakawa Y, Zing Conferences on Solid State Chemistry, Cancun, Mexico, 11 March 2008.

Complex Ordered Perovskites with Intriguing Physical properties: Shimakawa Y, MRS 2008 Satellite Meeting on Advanced Technologies for Advanced Characterizations of Advanced Materials, Beijing, China, 16 June 2008.

Charge and Orbital Orderings in Some New Oxides: Azuma M, UC Santa Barbara Workshop on Frontiers in Complex Oxides, Santa Barbara, USA, 6–12 July 2008.

$PbVO_3$ and $BiCoO_3$ with Large Tetragonal Distortions: Azuma M, 7th Korea-Japan Conference on Ferroelectricity, Jeju, Korea, 6–9 August 2008.

Grants

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

Azuma M, Search for Anomalous Magnetic, Electric and Dielectric Phenomena in Transition Metal Oxides with Active s-electrons, Grant-in-Aid for Scientific Research (B), 1 April 2007–31 March 2010.

International Research Center for Elements Science - Organotransition Metal Chemistry -

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

Prof
OZAWA, Fumiyuki
(D Eng)

Assoc Prof
OKAZAKI, Masaaki
(D Sc)

Assist Prof
TAKITA, Ryo
(D Pharm Sc)

Program-Specific Assist Prof
NAKAJIMA, Yumiko
(D Eng)

Res
WAKIOKA, Masayuki

Students

KIKUZAKI, Yuuta (M1)
MIYAGI, Kazuki (M1)
SHIRAISHI, Yu (M1)
KIMURA, Tetsuya (UG)
FUJITA, Daichi (UG)

Scope of Research

This laboratory aims at establishment of new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using experimental methods such as 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, (2) preparation of π-conjugated polymers by the use of well defined cross-coupling reactions, and (3) development of functional molecules including redox-active transition-metal clusters.

Research Activities (Year 2008)

Presentations

Catalytic Applications of Transition Metal Complexes Bearing Diphosphinidenecyclobutenes (DPCB-Y), Ozawa F, International Symposium on Chemistry Concerto Catalysis Based on Synergy of Elements, 12 July 2008, Rennes, France (Invited).

Electron-Induced Dynamic Behavior of [4Fe–4C] Cluster Core, Okazaki M, Takano M, Yoshimura K, Ozawa F, 38th International Conference on Coordination Chemistry, 24 July 2008, Jerusalem, Israel.

Grants

Ozawa F, Okazaki M, Takita R, Nakajima Y, Synergistic Effects of Transition Metals and Heavier Main Group Elements in Functional Organometallic Complexes, Grant-in-Aid for Priority Areas "Synergy of Elements", 1 September 2006–31 March 2010.

Ozawa F, Takita R, Nakajima, Y, Studies of Cross-coupling Reactions for Precise Synthesis of π- Conjugated Polymers, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Okazaki M, Mihara H, Construction of Novel Functional Molecules by Hybridization of Biomolecules with Transition Metal Clusters, Grant-in-Aid for Exploratory Research, 1 April 2007–31 March 2009.

Okazaki M, Design of Novel Catalysts Based on Redox-Active [4Fe–4C] Core, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Okazaki M, Construction of Functional Molecules Based on Characteristics of Polymetallic Cores, Grant-in-Aid for Scientific Research (B), 1 April 2008–31 March 2012.

Takita R, Development of Catalytic Reactions Using Low Coordinate Phosphine Ligands, Grant-in-Aid for Young Scientists (Start-up), 1 August 2007–31 March 2009.

Nakajima Y, Precise Design of Rare-earth Metal Based Catalysts Directed to Development of Novel Olefin Polymerization Process, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Award

Nakajima Y, Poster Prize ICOMCXXIII, Rennes, France, 14 July 2008.

Synthesis and Structures of Platinum(0) Alkyne Complexes with Extended π-Cojugated Systems

Organometallic complexes with extended π-conjugated systems have attracted continuous research interest because of their potential applications in material science. We recently found that 1,2-bis[(2,4,6-tri-*tert*-butylphenyl) phosphinidene]cyclobuta[*l*]phenanthrene (DPCB-phen) as a low-coordinated phosphorus ligand forms platinum(0) alkyne complexes with extended π-conjugated systems, [Pt(RCCR)(DPCB-phen)] [R = CO_2Me (**1a**), Ph (**1b**), C_6H_4-*p*-OMe (**1c**), C_6H_4-*p*-NMe_2 (**1d**)]. The colors of the complexes are highly dependent on alkyne ligands, showing a marked variation from reddish orange to teal.

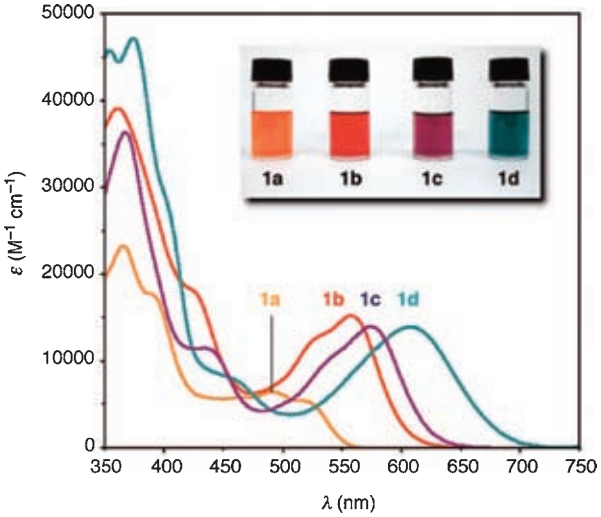


Figure 1. Absorption spectra of **1a-d** in $CHCl_3$.

Synthesis and Ligand Property of 1-Phosphaethenyl-2-phosphanylferrocenes

Novel bidentate-ligands with planar chirality, Fc (CH=PMes*)PAr_2 [Fc = ferrocene, Mes* = 2,4,6-tri-*tert*-buthylphenyl; PAr_2 = PPh_2 (**2a**), P(1-naphthyl)Ph (**2b**)], have been prepared for exploring the following points: (1) direct comparison of the ligand properties of phosphaalkene and phosphane, (2) application of phosphaalkene ligands to catalytic asymmetric reactions. Compounds **2a** and **2b** readily react with $[PtMe_2(\mu\text{-}SMe_2)]_2$ in Et_2O to afford dimethyl complexes with bidentate coordination of these ligands (**3a**, **3b**). The X-ray structure of **3b** indicates almost identical trans-influence of the phosphaethenyl and phosphanyl groups, showing comparable σ-donating abilities of those components. The complex [Pd(η^3-allyl)(**2a**)]OTf catalyzes hydroamination of 1,3-cyclohexadiene with aniline in toluene in the presence of molecular sieves 5A at room temperature, giving *N*-cyclohexen-3-ylaniline in 84% yield.

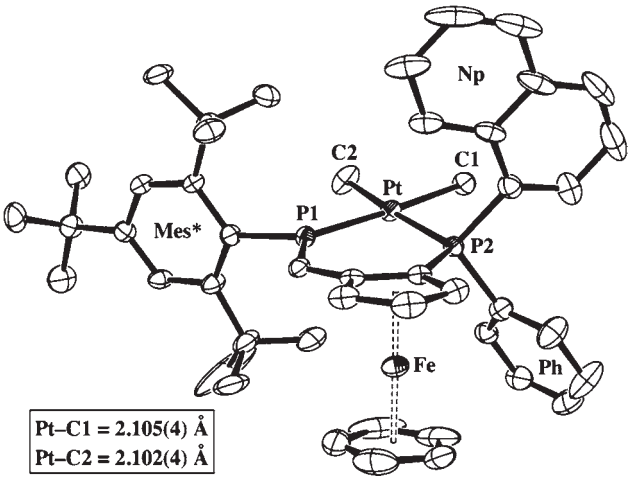
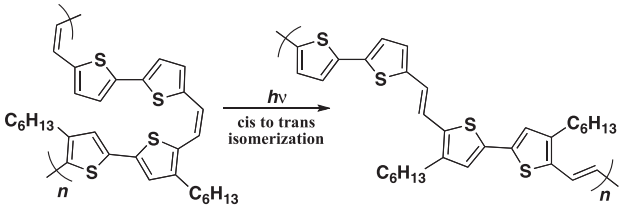


Figure 2. Molecular structure of **3b**. Hydrogen atoms are omitted for clarity.

Synthesis and Properties of All-cis Poly(arylene vinylene)s Containing Thiophene Cores

All-cis poly(arylene vinylene)s (PAV) containing thiophene units in the main chain have been prepared in highly stereocontrolled manner by Suzuki–Miyaura-type polycondensation. Thin films of all-cis PAVs, developed by spin-coating on quartz substrates, are insolubilized under UV-irradiation, along with cis–trans isomerization of the vinylene units. The photo-irradiated films exhibit relatively high carrier mobility up to 3.5×10^{-2} $cm^2/V{\cdot}s$, while the original films of all-cis PAVs are insulators.



Scheme 1. Photo-isomerization of all-cis poly(dithienylene vinylene).

International Research Center for Elements Science - Photonic Elements Science -

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

Prof
KANEMITSU, Yoshihiko
(D Eng)

Assoc Prof
MATSUDA, Kazunari
(D Eng)

Assist Prof
TAYAGAKI, Takeshi
(D Sc)

Assist Prof (SER)
YAMAMOTO, Shinpei
(D Eng)

PD
ITO, Hisashi
(D Sc)

SPD (JSPS)
MIYAUCHI, Yuhei
(D Eng)

PD
YAMADA, Yasuhiro
(D Sc)

Students

HIRANO, Daisuke (D2)
MATSUNAGA, Ryusuke (D1)
TAGUCHI, Seiji (M2)
YOSHIKAWA, Kohei (M2)
UEDA, Akihiro (M2)
SAKASHITA, Takerou (M1)
YAMAMOTO, Hidenobu (M1)

Visitor

ANTONIN, Fejfar — Institute of Physics, Academy of Sciencies of the Czech Republic, Czech Republic, 1 October 2007–31 March 2008

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 in semiconductor nanostructures.

Research Activities (Year 2008)

Publications

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).

Yasuda H, Kanemitsu Y: Dynamics of Nonlinear Blue Photoluminescence and Auger Recombination in $SrTiO_3$, *Phys. Rev. B*, **77**, [193202-1]-[193202-4] (2008).

Hirano D, Tayagaki T, Yamada Y, Kanemitsu Y: Dynamics of Biexciton Localization in $Al_xGa_{1-x}N$ Mixed Crystals under Exciton Resonant Excitation, *Phys. Rev. B*, **77**, [193203-1]-[193203-4] (2008).

Ueda A, Matsuda K, Tayagaki T, Kanemitsu Y: Carrier Multiplication in Carbon Nanotubes Studied by Femtosecond Pump-probe Spectroscopy, *Appl. Phys. Lett.*, **92**, [233105-1]-[233105-3] (2008).

Presentations

Mechanism of Carrier Multiplication in Carbon Nanotubes Studied by Ultrafast Pump-Probe Spectroscopy, Ueda A, Matsuda K, Tayagaki T, Kanemitsu Y, 8th International Conference on Excitonic Processes in Condensed Matter (EXCON08), 22–27 June 2008, Kyoto, Japan.

Excitonic Properties of Carbon Nanotubes Studied by Advanced Optical Spectroscopy, Matsuda K, The 5th Japan-Korea Symposium on Carbon Nanotube, 8–12 November 2008, Busan, Korea (Invited).

Direct Observations for Dark Excitons in Carbon Nanotubes due to the Aharonov-Bohm Effect

Electronic properties of single-walled carbon nanotubes (SWNTs) have attracted much attention from the fundamental physics viewpoint. The enhanced Coulomb interaction leads to the formation of stable 1-dimensional excitons in SWNTs. We studied exciton structures and the Aharonov-Bohm effect in a single carbon nanotube using micro-photoluminescence (PL) spectroscopy under magnetic field at low temperatures. A single sharp PL peak from the bright exciton state of a single carbon nanotube was observed under zero magnetic field, and the additional PL of dark exciton state appeared below the bright exciton peak under high magnetic fields as shown in Figure 1. It was found that the split between the bright and dark exciton states is several meV at zero field. The tube diameter dependence of the splitting arises from the intervalley short-range Coulomb interaction.

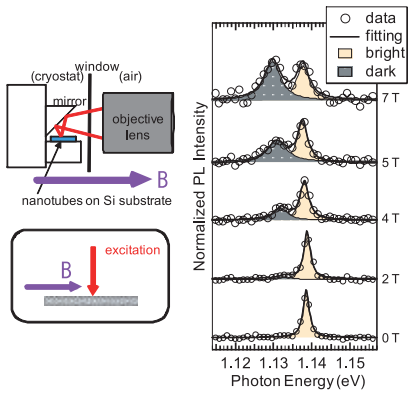


Figure 1. Schematic of experimental setup of a single nanotube spectroscopy under a magnetic field. PL spectra of a single carbon nanotube under magnetic fields.

Carrier Multiplication in Carbon Nanotubes

Carbon nanotubes are one of the excellent materials for studying the many-body effects of excitons, because of their unique band structures and large exciton binding energies. We studied exciton population dynamics in single-walled carbon nanotubes using pump-probe transient absorption spectroscopy. The temporal profiles of the transient absorption signals depend on the excitation intensity and excitation photon energy. We observed carrier multiplication in carbon nanotubes at room temperature, when the excitation photon energy exceeds the third subband exciton energy. We demonstrated that carbon nanotubes show unique optical responses because of their strong electron-electron interactions.

Direct and Stepwise Energy Transfer in Close-packed Metal and Semiconductor Nanoparticle Monolayer Films

Semiconductor and metal nanoparticles (NPs) serve as nanoscale building blocks for tailored materials with fascinating multifunctional properties beyond those of bulk crystals. Recently, we prepared macroscopically ordered NP supra-solids and close-packed NP solids have been prepared, allowing the study of quantum and cooperative phenomena. One of the central issues in ordered or close-packed NP solids is the understanding of energy and charge transfer processes on a nanoscale. We studied the dynamics of PL and energy transfer in close-packed monolayer films of CdSe and Au NPs assembled using the Langmuir–Blodgett technique. The PL intensity and dynamics depend on the ratio of CdSe to Au NPs in the mixed films in Figure 2. The PL quenching of CdSe NPs occurs through rapid energy transfer from excitons in CdSe NPs to plasmons in Au NPs. The PL decay curves of the mixed NPs monolayers are determined by three decay processes: the direct energy transfer between the nearest-neighbor CdSe and Au NPs (CdSe→Au), the stepwise energy transfer from CdSe to CdSe to Au NPs (CdSe→CdSe →Au), and the radiative recombination in CdSe NPs.

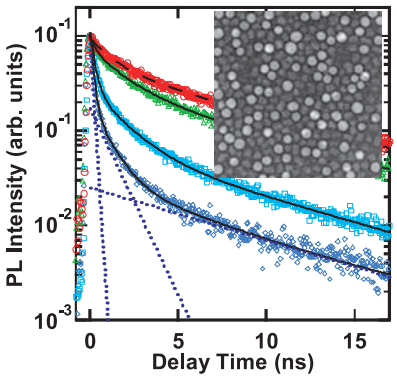


Figure 2. PL dynamics in CdSe and Au NPs monolayer films in various mixing ratios. Inset shows the TEM image of the CdSe and Au NPs mixed monolayer film.

Grants

Kanemitsu Y, Study of Highly Excited State in Semiconductor Nanostructures by Means of Time and Spatially Resolved Spectroscopy, Grant-in-Aid for Scientific Research (B), 1 April 2006–31 March 2008.

Matsuda K, Optical Quantum State Manipulation of Carbon Nanotubes, Grant-in-Aid for Scientific Research (B), 1 April 2008–31 March 2011.

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- Bioknowledge Systems -

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Prof
KANEHISA, Minoru
(D Sc)

Assoc Prof
GOTO, Susumu
(D Eng)

Assist Prof
HATTORI, Masahiro
(D Sc)

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

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

Program-Specific Res
HAYES, Nelson
(Ph D)

Program-Specific Res
HU, Qian-Nan
(Ph D)

PD
RUIZ, Diego Deiz
(Ph D)

Researchers

HIRAKAWA, Mika
MORIYA, Yuki
NAKAGAWA, Zenichi
SANO, Etsuko

Research Associates (pt)

SAKIYAMA, Tadahiro
SHIGEMIZU, Daichi

Students

ONUKI, Ritsuko (D3)
HONDA, Wataru (D3)
HASHIMOTO, Kosuke (D3)
MUTO, Ai (D3)
SUGA, Akitsugu (D3)
TANAKA, Michihiro (D2)
TAKARABE, Masataka (D2)
SHIMIZU, Yugo (D1)
DONG, Hong Ju (D1)
MIZUTANI, Sayaka (M2)
HIRANUKA, Kazushi (M2)
KOBAYASHI, Takeshi (M2)
NISHIMURA, Yosuke (M1)
ERGUNER, Bekir (M1)
JIN, Zhao (RS)
KONG, Xiang Shuo (UG)

Scope of Research

DNA, RNA, and proteins are the basic molecular building blocks of life, but the living cell contains additional molecules, including water, ions, small chemical compounds, glycans, lipids, and other biochemical molecules, without which the cell would not function. Because the proteins responsible for biosynthesis, biodegradation, and transport of these additional molecules are encoded in the genome, one may assert that all cellular functions are specified by the genomic DNA sequence. In practice, however, it is not possible to infer higher-level systemic functions of the cell or the organism simply from the molecular sequence infomation alone. 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 for practical applications in medical and pharmaceutical sciences.

Research Activities (Year 2008)

Grants

Kanehisa M, Knowledge Information Infrastructure for Genome Information Science, Kyoto University 21st Century COE Program, MEXT.

Kanehisa M, Backbone Database for Analysis of the Biological Systems and Environment, Grant-in-Aid for Scientific Research on Priority Areas, MEXT.

Kanehisa M, Deciphering Systemic Biological Functions by Integration of Genomic and Environmental Information, Bioinformatics Research and Development, JST.

KEGG PLANT Database

Plants produce vast and diverse natural products. These natural products are important for our lives because of their great utility as drugs and industrial materials (fibers, oils, dyes, perfumes etc.). Plants are also a major source of crude drugs. In this context, plant natural products and their biosynthetic pathways have been studied by plant scientists extensively for a long time. Recently, in the post genomic era, plant metabolomics is an important technology for plant omics research. An integrated resource of pathway and metabolite databases focused on plants is especially important for this research field.

KEGG PLANT is a new interface to the KEGG database resource, which contains an overview pathway map and sub-category pathway maps to summarize plant pathways, and hierarchical classification of plant secondary metabolites and semi-synthetic drugs from plant origin. Plant secondary metabolite pathways in KEGG PATWAY database are also extensively updated and linked to the overview and subcategory maps. Also KEGG PLANT information is linked to some KEGG DRUG compound data via hierarchical classification of semi-synthetic drugs. This useful information will help plant research and related application research field.

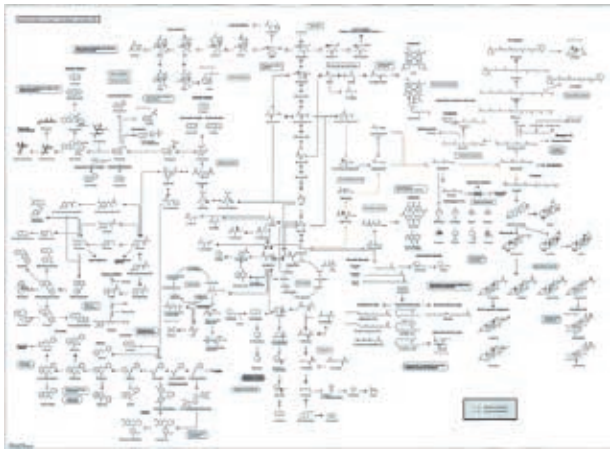

Figure 1. The KEGG PLANT Overview Map.

From the Repertoire of Desaturases and Elongases to Fatty Acid Variations

The repertoire of biosynthetic enzymes found in an organism is an important clue for elucidating the chemical structural variations of various compounds. In the case of fatty acids, it is essential to examine key enzymes that are desaturases and elongases, whose combination determine the range of fatty acid structures.

We obtained 275 desaturase and 265 elongase homologs from 56 eukaryotic genomes using PSI-BLAST. Phylogenetic and motif analysis indicated that the desaturases consist of four functionally distinct subfamilies, and the elongases consist of two subfamilies. Each subfamily has a distinct motif, whose profiles can be used for functional assignments of desaturases and elongases in newly sequenced genomes. We then predicted the ability to synthesize fatty acids, especially six types of fatty acids widely distributed in nature from the pathway view point (Figure 2). Consequently, we found that the ranges of synthesizable fatty acids are often different even between closely related organisms. The reason is that, as well as diverging into subfamilies, the enzymes have functionally diverged within the individual subfamilies. Such a variety of fatty acids may contribute to adaptation to individual environments and the ability to synthesize specific metabolites. This study provides an example of a potent strategy to bridge the gap from genomic knowledge to chemical knowledge.

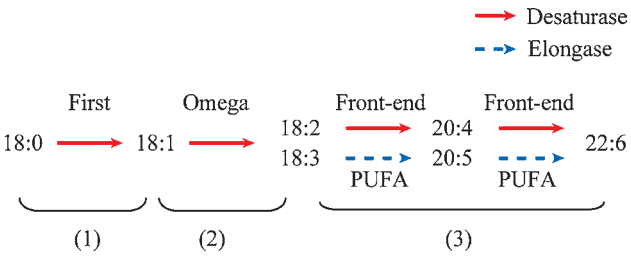

Figure 2. A schematic pathway of unsaturated fatty acids with subfamily enzymes. (1) The pathway from stearic acid (18:0) to oleic acid (18:1), catalyzed by the First subfamily. (2) The pathway from oleic acid (18:1) to linoleic acid (18:2) and alpha-linolenic acid (18:3), catalyzed by the Omega subfamily. (3) The pathway from oleic acid (18:1) and linoleic acid (18:2) to DHA (22:6), catalyzed by the Front-end subfamily the PUFA subfamily.

Kanehisa M, Integration of Genomics and Chemistry in Glycome Informatics, NIH, USA.

Goto S, Hierarchical Structuring and Integration of Knowledge in Life Sciences, Integrated Database Project, MEXT.

Bioinformatics Center
- Biological Information Networks -

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

Prof
AKUTSU, Tatsuya
(D Eng)

Assist Prof
HAYASHIDA, Morihiro
(D Inf)

Assist Prof
TAMURA, Takeyuki
(D Inf)

Program-Specific Res
KATO, Yuki
(D Eng)

Guest Res Assoc
SONG, Jiangning
(Ph D)

Students

MOURI, Kazunari (D3)
BROWN, John (D2)
POOLSAP, Unyanee (D1)
NARITA, Yuki (M1)

Visitor

TAN, Hao Monash University, Australia, 7 December 2007–1 March 2008

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.

Research Activities (Year 2008)

Publications

Hayashida M, Tamura T, Akutsu T, Zhang SQ, Ching WK: Algorithms and Complexity Analyses for Control of Singleton Attractors in Boolean Networks, *EURASIP J Bioinform Syst Biol*, **2008**, [521407-1]-[521407-16] (2008).

Fujiwara H, Wang J, Zhao L, Nagamochi H, Akutsu T: Enumerating Treelike Chemical Graphs with Given Path Frequency, *J. Chem. Inf. Model*, **48**, 1345-1357 (2008).

Song J, Tan H, Takemoto K, Akutsu T: HSEpred: Predict Half-sphere Exposure from Protein Sequences, *Bioinformatics*, **24**, 1489-1497 (2008).

Presentations

An Improved Algorithm for Detecting a Singleton Attractor in a Boolean Network Consisting of AND/OR Nodes, Tamura T, Akutsu T, 3rd International Conference on Algebraic Biology, 31 July 2008.

Prediction of Protein Beta-Sheets: Dynamic Programming versus Grammatical Approach, Kato Y, Akutsu T, Seki H (Nara Institute of Science and Technology), 3rd IAPR International Conference on Pattern Recognition in Bioinformatics (PRIB2008), 15 October 2008.

On Distribution and Enumeration of Attractors in Probabilistic Boolean Networks, Hayashida M, Tamura T, Akutsu T, Ching WK (The University of Hong Kong), The 2nd International Symposium on Optimization and Systems Biology, 1 November 2008.

Grants

Akutsu T, Goto S, Mochizuki A, Tokita K, Mathematical Analysis of Structure and Dynamics of Biological Information Networks, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2005–31 March 2010.

Akutsu T, Kawabata T, Nagamochi H, Hayashida M, A Novel Approach to Computational Drug Design Based on Graph Theory and Kernel Methods, Grant-in-Aid for Scientific Research(A), 1 April 2007–31 March 2011.

Akutsu T, Data Compression Based Approach to Elucidation of Principles of Complex Biological Systems, Grant-in-Aid for Exploratory Research, 1 April 2007–31 March 2009.

Topics

Emergence of Scale-free Distribution in Protein-protein Interaction Networks based on Random Selection of Interacting Domain Pairs

Recent researches for biological and artificial networks have uncovered common network architecture, called scale-free topology. The origin of the scale-free topology has been explained using growth and preferential attachment mechanisms. In a cell, proteins are the most important carriers of functions, and are contain domains as elemental units responsible for the physical interaction between protein pairs.

We propose a model for protein-protein interaction networks that reveals the emergence of two possible topologies. We show that depending on the number of randomly selected interacting domain pairs, the connectivity distribution follows either a scale-free distribution, even in the absence of the preferential attachment, or a normal distribution. This new approach only requires an evolutionary model of proteins (nodes) but not for the interactions (edges). The edges are added by means of random interaction of domain pairs. As a result, this model offers a new mechanistic explanation for understanding complex networks with a direct biological interpretation because only protein structures and their functions evolved through genetic modifications of amino acid sequences. These findings are supported by numerical simulations using *H. sapiens* protein domain data from UniProt database.

Nacher JC, Hayashida M, Akutsu T: *BioSystems*, in press.

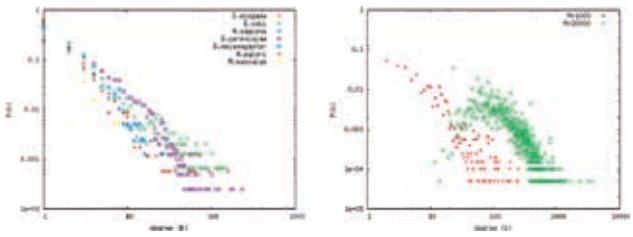

Figure 1. Degree distribution $P(k)$ of PPI networks (Left) real data for several organisms (Right) simulated data using *H. sapiens* data for the number of randomly selected interacting domain pairs, N =1000, 30000. A power-law distribution and a normal distribution were respectively observed.

Prediction of RNA Secondary Structure with Pseudoknots Using Integer Programming

RNA secondary structure prediction is one major task in bioinformatics, and various computational methods have been proposed so far. Pseudoknot is one of the typical substructures appearing in several RNAs, and plays an important role in a number of RNA functions such as ribosomal frameshifting and splicing. Prediction of RNA secondary structure with pseudoknots is still challenging since the problem is NP-hard when arbitrary pseudoknots are taken into consideration.

We propose a new method of predicting RNA secondary structure with pseudoknots based on integer programming. In our formulation, we aim at minimizing the value of the objective function that reflects free energy of a folding structure of an input RNA sequence since many single-stranded RNAs are considered to fold back on themselves to be thermodynamically stable. We focus on a practical class of pseudoknots by setting constraints appropriately. Experimental results for a set of real RNA sequences show that our proposed method outperforms several existing methods in sensitivity. Furthermore, for a set of sequences of small length, our approach achieved good performance in both sensitivity and specificity. Our integer programming-based approach to RNA secondary structure prediction is flexible and extensible enough to describe various types of secondary structures.

Poolsap U, Kato Y, Akutsu T: *BMC Bioinformatics*, 10 (Suppl 1) (2009).

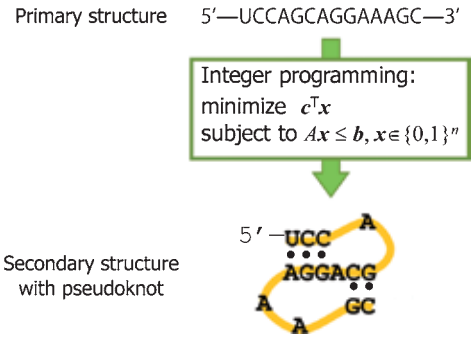

Figure 2. Prediction of RNA pseudoknotted structure.

Awards

Kato Y, IPSJ Best Paper Award, RNA Pseudoknotted Structure Prediction Using Stochastic Multiple Context-Free Grammar, Information Processing Society of Japan, 30 May 2008.

Kato Y, SIGBIO Best Paper Award, RNA Pseudoknotted Structure Prediction Using Stochastic Multiple Context-Free Grammar, Information Processing Society of Japan (Bioinformatics and Genomics), 17 December 2008.

Bioinformatics Center
- Pathway Engineering -

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

Prof
MAMITSUKA, Hiroshi
(D Sc)

Assist Prof
TAKIGAWA, Ichigaku
(D Eng)

Assist Prof*
SHIGA, Motoki
(D Eng)

*Bioinformatics Center, Laboratory of Advanced Data Mining for Bioinformatics

Program-Specific Res
KAYANO, Mitsunori
(D Sc)

Program-Specific Res
NATSUME, Yayoi
(D Agr)

Program-Specific Res
WAN, Raymond
(Ph D)

PD (JSPS)
HANCOCK, Timothy Peter
(Ph D)

Students

MATSUSHIMA, Yoshifumi (M2)
SATO, Yoshiko (M2)

Visitors

Prof WONG, Limsoon	National University of Singapore, Singapore, 14 January 2008
DU VERLE, David	Pierre & Marie Curie University, France, 21 May 2008/1 September 2008
Dr VO, Anh Ngoc	University of Melbourne, Australia, 22 June–20 July 2008
KOH, Chuan Hock	National University of Singapore, Singapore, 7 November 2008
Assoc Prof SJÖLANDER, Kimmen	University of California, Berkeley, USA, 10–11 November 2008

Scope of Research

With the recent advancement of experimental techniques in molecular biology, research in modern life science is shifting to the comprehensive understanding of a biological mechanism consisting of a variety of molecules. Our focus is placed on molecular mechanisms in biological phenomena, represented by biological networks such as metabolic and signal transduction pathways. Our research objective is to develop techniques based on computer science and/or statistics to systematically understand biological entities at the cellular and organism level.

Research Activities (Year 2008)

Publication

Hashimoto K, Takigawa I, Shiga M, Kanehisa M, Mamitsuka H: Mining Significant Tree Patterns in Carbohydrate Sugar Chains. *Bioinformatics*, **24 (16)** (*Proceedings of the Seventh European Conference on Computational Biology (ECCB 2008)*, Cagliari, Sardinia-Italy, September 2008), i167-i173, 2008.

Presentations

Data-integrative Informatics for Chemical Genomics, Mamitsuka H, Keynote Speech, *Workshop: Systems Biology –From Molecules to Life–,* La Trobe University, Melbourne, Australia, 27 May 2008.

Clustering Numerical Vectors with a Modularity Network, Mamitsuka H, Invited Talk, *Foundation of Computational Mathematics (FoCM) 2008*, City University of Hong Kong, China, 22 June 2008.

Mining Significant Patterns from Trees, Mamitsuka H, Invited Talk, *Hayama Seminar*, Sokendai, Hayama, Japan, 14 October 2008.

Efficiently Finding Significant Substructural Patterns Conserved in Glycans, Takigawa I, *Annual Conference of the*

Efficiently Mining Significant Substructural Patterns Conserved in Glycans

Glycans or carbohydrate sugar chains are one of the four fundamental macromolecular components of all cells along with nucleic acids, proteins, and lipids. Most of glycans are on the outer surface of cellular and secreted macromolecules, and modulate or mediate a wide variety of events in cell-cell and cell-matrix interactions crucial to the development and function of a complex multicellular organism. The structure of a glycan is a branched (or a linear) chain of monosaccharides attached to one another via glycosidic linkages. These "tree-shaped" sequence structures potentially lead to considerably more linkage variation in contrast to a linear sequence such as nucleic acids and proteins. However, naturally occurring ones contain relatively few of the possible monosaccharide units in a limited number of combinations. Thus, as with sequence motifs in nucleic acids or proteins, conserved structural patterns in glycans can be a key for analyzing functions of glycans. With the rapid increase in glycan structural data, mining conserved patterns from large-scale data is vital to make better understandings of glycans.

The techniques for finding all frequent subtree patterns in a given set of trees have been developed in the field of data mining. However, complete enumeration of frequent subtrees practically generates a huge number of outputs, which makes subsequent biological analysis difficult. The output patterns, hence, should be summarized as more compact patterns keeping characteristic information. For example, CMTreeMiner can retrieve closed and maximal subtree patterns. In our preliminary trials with real glycan data, the closed patterns produced still large outputs and the maximal patterns contained only too specific patterns. Moreover, very frequent patterns were often not biologically significant because such patterns were likely to be too simple and could be ubiquitous simply by chance. In order to handle these two types of problems, we first introduce a new concept, α-closed frequent subtrees, as parametric summarization of patterns controlled by α, and develop an efficient method for mining all these subtree patterns from given trees. Then we rank these obtained patterns according to not the frequencies but the *p*-values in a significance test against random control data. We experimentally verified the effectiveness of this approach using real structures of glycans retrieved from KEGG GLYCAN database. As shown in Table 1, we examined the top ranking subtrees obtained by our method and confirmed that those subtrees are significant motifs in glycobiology such as typical core structures, known extension patterns, and functionally important subtree motifs.

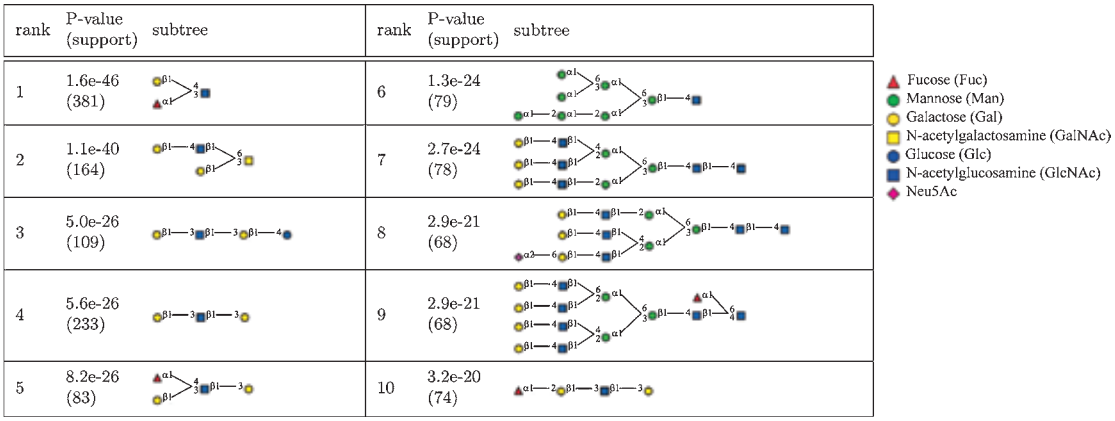

Figure 1. Top ten significant patterns in glycans.

Japanese Society for Bioinformatics (JSBi2008), Senri Life Science Center, Osaka, Japan, 15 December 2008.

Grants

Mamitsuka H, Integrative Data Mining Approaches for Unstructured Data in Life Sciences, Research Grant from BIRD (BioInformatics Research and Development) of JST (Japan Science and Technology Agency), 15 October 2007–30 September 2010.

Takigawa I, Multifaceted Exploration of Nonhomogeneous and Ambiguous Data by Combining Partial Similarities, Grant-in-Aid for Young Scientist (B), 1 April 2008–31 March 2011.

Shiga M, Integrative Data Mining Based on Structure Analysis of Biological Networks, Grant-in-Aid for Young Scientist (B), 1 April 2008–31 March 2010.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
NOZAKI, Kyoko
(D Eng)

Laboratory of Polymer Controlled Synthesis
Professor, Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo
(7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656)

Lecture at *ICR*
Polymerization of Polar Monomers Using Late Transition Metal Catalysts

Vis Prof
ITO, Susumu
(D Agr)

Laboratory of Molecular Microbial Science
Professor, Creative Research Initiative "Sousei"
Hokkaido University
(Kita 21, Nishi 10, Kita-ku, Sapporo 001-0021)

Lecture at *ICR*
Exploration and Application of Microbial Enzymes

Vis Prof
MITSUOKA, Kaoru
(D Sc)

Laboratory of Structural Molecular Biology
Team Leader, Protein Structural Information Analysis Team, Biomedicinal Information Research Center, National Institute of Advanced Industrial Science and Technology
(2-42 Aomi, Koto-ku, Tokyo 135-0064)

Lecture at *ICR*
Cryo-Electron Microscopic Analyses of 3D-Structures of Membrane Proteins

Vis Prof
HORIMOTO, Katsuhisa
(D Sc)

Laboratory of Biological Information Networks
Leader, Biological Network Team, Computational Biology Research Center, Advanced Industrial Science and Technology
(AIST Tokyo Waterfront Bio-IT Research Building, 2-42 Aomi, Koto-ku, Tokyo, 135-0064)

Lecture at *ICR*
Analysis of Dynamics of Biological Networks Using Symbolic Computation

Vis Prof
BUCKEL, Wolfgang
(Ph D)

Laboratory of Molecular Microbial Science
Professor, Microbiology, Philipps-University Marburg
(Karl-von-Frisch Strasse 8, D-35043 Marburg, Germany)

Lecture at *ICR*
Studies of Catalytic Mechanisms of Enzymes Containing Transition Metals

Vis Prof
KOTORA, Martin
(Ph D)

Laboratory of Organic Main Group Chemistry
Professor, Department of Organic and Nuclear Chemistry, and Centre for New Antivirals and Antineoplastics, Faculty of Science, Charles University
(Hlavova 8, 128 43 Praha 2, Czech Republic)

Lecture at *ICR*
Synthesis of Estrone Based on Organometallic Reactions

Vis Assoc Prof
MINOURA, Mao
(D Sc)

Laboratory of Organoelement Chemistry
Associate Professor, Department of Chemistry, School of Science, Kitasato University
(1-15-1 Kitasato, Sagamihara, Kanagawa 228-8555)

Lecture at *ICR*
Synthesis and Structure of Hypervalent Organotellurium Compounds: How Many Chemical Bonds Can a Tellurium Form?

Vis Assoc Prof
HARADA, Kazuo
(D Sc)

Laboratory of Biofunctional Design-Chemistry
Associate Professor, Department of Life Science, Tokyo Gakugei University
(Koganei, Tokyo 184-8501)

Lecture at *ICR*
Combinatorial Analysis of RNA-Peptide Interaction

Vis Assoc Prof
AHN, Kyung Hyun
(D Eng)

Laboratory of Molecular Rheology
Associate Professor, School of Chemical and Biological Engineering, Seoul National University
(Seoul 151-744, South Korea)

Vis Assoc Prof
OKUNO, Tsuyoshi
(D Sc)

Laboratory of Photonic Elements Science
Associate Professor, Department of Applied Physics and Chemistry, The University of Electro-Communications
(Chofu, Tokyo 182-8585 Japan)

Lecture at *ICR*
Optical Properties of Rare-earth Ion Doped Semiconductor Nano-structures

Prof Em FUKUDA, Takeshi (D Eng)

Appointed as Res (pt) at ICR,
1 April 2008–31 March 2009

ICR-invited Professor
MARRUCCI, Giuseppe (PhD)
Certified, 9 April 2008

Professor, Università degli studi di Napoli "Federico II"
(Piazzale Tecchio 80, 80125 Napoli, Italy)

PERSONAL

Retirement

Professor NAKAHARA, Masaru
Division of Environmental Chemistry
—Solution and Interface Chemistry—

On 31 March, 2009, Dr. Masaru Nakahara retired from Kyoto University after 36 years of service was honored with the title of Professor Emeritus of Kyoto University. Dr. Nakahara was born in Ohshima Island, Yamaguchi Prefecture on 9 June, 1945. He graduated from Department of Chemistry, Faculty of Science, Kyoto University in 1968 and studied high-pressure physical chemistry in the Graduate School of Science under the supervision of late Professor Jiro Osugi. In 1974, he was granted the doctoral degree for the thesis entitled "Effects of pressure on the mobilities and hydration of Bu_4N^+, Me_4N^+, K^+, Cl^- ions". In 1973, he was appointed Research Associate in Department of Chemistry, Faculty of Science, Kyoto University, and in 1986 he was promoted to Associate Professor. In 1994, he was appointed Professor in the Institute for Chemical Research, Kyoto University and directed the Laboratory of Solution and Interface.

Through his academic career, Dr. Nakahara devoted himself to physical chemistry of solutions and interfaces, focusing on structure, dynamics, and reaction of water and aqueous solutions over a wide range of thermodynamic conditions. He first studied the ionic conductivity in solution. He clarified the validity and limitations of the dielectric friction theory and deepened the concept of Walden product. He then turned to NMR studies of solutions, notably in dilution conditions. He successfully examined the "solitary water" in organic solvents; it is an isolated water molecule without hydrogen bonding and the behavior of water in hydrophobic media was first revealed.

At the Institute for Chemical Research, he extended his study to high-temperature and/or high-pressure, extreme conditions. As a world pioneer, he first developed a high-temperature NMR probe and made possible the chemical-shift measurement at 400 °C. He revealed the persistence of hydrogen bonding in supercritical water and determined quantitatively the degree of hydrogen bonding in hot water. The dynamic picture of supercritical water was also established, and the molecular mechanism of the translational and rotational relaxations was finely clarified with the notion of solvation-shell lifetime.

With deep knowledge of hydration in hot water, he systematically investigated environmentally friendly reactions in supercritical water. He discovered several, non-catalytic C1 reactions, and clarified the general reaction pathways of aldehyde in hot water. The role of formic acid as an intermediate of the water-gas-shift reaction was pointed out, and this finding has led to a new scheme of hydrogen technology. The finding met the foundation of the new laboratory of Water Chemistry Energy in the Institute financially supported by AGC.

Dr. Nakahara's scientific achievements were published in 176 original papers. He was frequently invited to prestigious international conferences such as Gordon Conference (1988 and 1998), EuroConference (2001), and The International Conference on the Properties of Water and Steam (2004). To his achievements, the Award of The Japan Society of High-Pressure Science and Technology was given in 2004.

Dr. Nakahara's contribution to scientific communities is also to be noted. He has served as President of The Japan Society of High-Pressure Science and Technology (2001) and as President of The Japan Association of Solution Chemistry (2004 to the present), and was involved in organizing international conferences such as The 26th International Conference on Solution Chemistry (1999), The 14th International Conference on the Properties of Water and Steam (2004), and The 1st International Conference of the Grand Challenge to Next-Generation Integrated Nanoscience (2008). He was active in a number of committees of governmental sectors including MEXT, METI, and JSPS.

Dr. Nakahara's contribution to Kyoto University and the Institute though his scientific, educational, and administrative activities is hereby greatly acknowledged.

Awards

MIZUHATA, Yoshiyuki

Mitsubishi Kagaku Award in Synthetic Organic Chemistry, Japan

"Construction of Aromatic Compounds Having Plural Heavier Group 14 Elements and Their Application to the Functional Materials"

The Society of Synthetic Organic Chemistry, Japan

20 February 2008

GOTO, Atsushi

Young Scientist Presentation Award

54th Annual Kobe Polymer Research Symposium
"A Novel Class of Living Radical Polymerization with Typical Element Catalysts – Reversible Chain Transfer Catalyzed Polymerization"

The Society of Polymer Science, Japan

18 July 2008

ICR Award for Young Scientists

"Reversible Chain Transfer Catalyzed Polymerization (RTCP): A New Class of Living Radical Polymerization"

Institute for Chemical Research, Kyoto University

5 December 2008

TAKAHASHI, Masahide

Award for Promising Young Researchers

"Fabrication of Microstructures Using Photo-activated Processes"

The Ceramics Society of Japan, Kansai Branch

24 July 2008

ONO, Teruo

FFIT Prize

"Development of the Magnetization Control Technology by Electric Currents"

Funai Foundation for Information Technology

19 April 2008

The 10th Sir Martin Wood Prize

"Magnetization Control in Nano-Magnets by Electric Currents"

Millennium Science Forum

12 November 2008

Japan IBM Prize

"Research on the Magnetization Control by Spin-polarized Currents"

IBM Japan

26 November 2008

MATUBAYASI, Nobuyuki

Award for Distinguished Achievement and Nose Memorial Award

"Numerical Methods for Rotational Equation of Motion and Free-Energy Calculations Based upon Solution Theory: New Developments and Applications"

The Japan Society of Molecular Simulation

18 November 2008

HARUTA, Mitsutaka

ICR Award for Graduate Students

"Atomic Resolution ADF-STEM Imaging of Organic Molecular Crystal of Halogenated Copper Phthalocyanine"

Institute for Chemical Research, Kyoto University

5 December 2008

Paper Awards

WATANABE, Hiroshi

The Award of the Society of Polymer Science, Japan

The 57th Annual Meeting of the Society of Polymer Science, Japan
"Molecular Dynamics and Rheology of Homogeneous and Inhomogeneous Polymer Liquids"

The Society of Polymer Science, Japan

29 May 2008

KASAI, Shinya

Young Author Best Presentation Awards
Oyo Butsuri Gakkai

"Time-resolved Measurement of the Current-induced Vortex Core Dynamics in a Ferromagnetic Circular Disk"

The Japan Society of Applied Physics

29 March 2008

TAKAYA, Hikaru

The Presentation Award for Young Chemists

The 88th Annual Meeting of the Chemical Society of Japan, Tokyo
"Programmable Metal Unit Arrangement on Peptides to Create Combination and Configuration-Controlled Organometallic Materials"

The Chemical Society of Japan

29 March 2008

HASHISAKA, Masayuki

IUPAP Young Author Best Paper Awards

The International Conference on the Physics of Semiconductors
"Bolometric Shot Noise Detection in Coupled Quantum Point Contacts"

International Union of Pure and Applied Physics

1 August 2008

MATSUNAGA, Ryusuke

ICR Award for Graduate Students

"Evidence for Dark Excitons in a Single Carbon Nanotube due to the Aharonov-Bohm Effect"

Institute for Chemical Research, Kyoto University

5 December 2008

Award for Encouragement of Research in Condensed Matter Photophysics

"Magneto-Photoluminescence Spectroscopy of Single Carbon Nanotubes: Direct Observation of Dark Excitons"

11 December 2008

TAKAHASHI, Hideaki

SRJ Paper Award

The 35th Annual Meeting of SRJ
"Viscoelastic Behavior of Scarcely Crosslinked Poly(dimethyl siloxane) Gel"

The Society of Rheology, Japan

14 May 2008

KOSHINO, Masanori

KURATA, Hiroki

ISODA, Seiji


Microscopy and Microanalysis, 2007 Best Materials Paper Award

"Stability Due to Peripheral Halogenation in Phthalocyanine Complexes"

Microscopy Society of America

10 September 2008

KATO, Yuki

IPSJ Best Paper Award

"RNA Pseudoknotted Structure Prediction Using Stochastic Multiple Context-Free Grammar"

Information Processing Society of Japan

30 May 2008

SIGBIO Best Paper Award

"RNA Pseudoknotted Structure Prediction Using Stochastic Multiple Context-Free Grammar"

Information Processing Society of Japan (Bioinformatics and Genomics)

17 December 2008

KAYANO, Mitsunori

JSAS Prize

"Functional Principal Component Analysis via Regularized Basis Expansion and Its Application"

Japanese Society of Applied Statistics (JSAS)

7 June 2008

Poster Awards

TANABE, Taro

Best Poster Award

The 2nd Asian Silicon Symposium/The 15th International Symposium on Organosilicon Chemistry
"Silanedichalcogenolato Transiton Metal Complexes: Structures, Properties, and Their Unique Reactivities"

ISOS-XV Organizing Committee

6 June 2008

YUASA, Akihiro

Best Poster Award

55th Symposium on Organometallic Chemistry, Japan
"Synthesis, Structure, and Properties of Ferrocenyl- and Ruthenocenyl-disilenes"

The Kinki Chemical Society, Japan

19 December 2008

TANABE, Yusuke

Best Poster Award

55th Symposium on Organometallic Chemistry, Japan
"Structures and Properties of the Hydration Product of Silabenzene–$Cr(CO)_3$ Complex and Related Compounds"

The Kinki Chemical Society, Japan

19 December 2008

IMAMURA, Yoko

Best Poster Award

2nd Symposium on Organic π-Electron Systems
"Colorimetric High-sensitive Recognition of Spermidine and Spermine"

5 December 2008

IMANISHI, Miki

The Best Poster Prize

Chemistry in the New World of Bioengineering and Synthetic Biology
"Artificial Zinc Finger-Type Transcription Factors Targeting Circadian Clock Genes"

Royal Society of Chemistry, UK

24 September 2008

AKI, Shiori

The Best Poster Award

ZOMES-V (The Fifth International Symposium on the COP9 Signalosome, Proteasome and eIF3: At the Interface between Signaling & Proteolysis)
"COP9 Signalosome Interacts with RNA Processing Factors in Arabidopsis"

Organizing Committee of ZOMES-V

13 November 2008

TANAKA, Kentaro

The Best Poster Presentation Award (Good Discussion)

The 39th Summer School of the Society of Fiber Science and Technology, Japan
"Critical Ionic Strength for Chitosan Aqueous Solution"

The Society of Fiber Science and Technology, Japan

11 September 2008

ITO, Chie

Poster Prize

8th Annual Meeting of the Japanese Society for Neutron Science
"Shish-kebab Structural Analysis for Drawing with Small-Angle Neutron Scattering Measurement"

2 December 2008

IWAMOTO, Tatsuya

The SRJ Best Presentation Award

The 35th Annual Meeting of SRJ
"Dielectric Relaxation of Guest Homopolyisoprene Constrained in Microdomain Formed by Styrene-Isoprene-Styrene Triblock Copolymer"

The Society of Rheology, Japan

14 May 2008

YAMADA, Masako

Poster Prize

8th Annual Meeting of the Japanese Society for Neutron Science
"Development of the Permanent Magnet Sextupole Lens for Focusing of Pulsed Neutron Beam"

2 December 2008

NAKAJIMA, Yumiko

Poster Prize ICOMC 2008

XXIII International Conference on Organometallic Chemistry
"Rare-earth Metal/Platinum Heterobinuclear Complexes: Synthesis and Reactivity Investigation"

13–18 July 2008

UEDA, Akihiro

Mitsubishi Electric Prize for Young Poster Presenter

The 8th International Conference on Excitonic Processes in Condensed Matter (EXCON'08)
"Mechanism of Carrier Multiplication in Carbon Nanotubes Studied by Ultrafast Pump-Probe Spectroscopy"

27 June 2008

Obituary

Professor Emeritus

Dr. TAKEZAKI, Yoshimasa (1917–2008)

Dr. Yoshimasa Takezaki, Professor Emeritus of Kyoto University, passed away on July 9, 2008.

Dr. Takezaki was born in Osaka on September 28, 1917. He graduated from Kyoto Imperial University with a major in Chemistry in 1940. In April of the same year, he joined the Institute for Chemical Research (ICR), Kyoto Imperial University as a researcher and as an Assistant Professor in June of the same year. In September of the same year, he moved to naval arsenal as an engineer officer and was there until September 1945. In February 1946, he was appointed a Lecturer in the Faculty of Engineering, Kyoto Imperial University. In November 1947, he joined ICR, Kyoto University as Associate Professor, and was promoted to Full Professor at Kyoto University in March 1951 to direct the Laboratory of High Pressure Chemistry. He retired from Kyoto University in 1981 and subsequently was honored with the title of Professor Emeritus of Kyoto University.

He conducted extensive research in photochemistry and high-pressure chemistry. He developed novel addition reactions of carbon monoxide and carbon dioxide to various organic compounds. These reactions made it possible to construct novel carbon framework of organic compounds which were very important from both scientific and industrial points of view. He also contributed significantly to the progress in understanding the mechanism on combustion processes involving free radicals. Especially, he systematically performed kinetic studies on reactions of methyl radical generated from pyrolysis of azomethane with various oxygen-including organic compounds such as alcohols, aldehydes, ketones, and ethers, which gave us great insight into the correlations between oxidative chain reactions and knocking characteristics. He was a pioneer in the research of reactive intermediates generated by photochemical process and their reactions. His achievements in each field are highly appreciated internationally as well as domestically.

He gave lectures on physical chemistry at the Graduate School of Engineering, Kyoto University as well as at many other foreign and domestic institutions, and supervised the dissertation studies of a number of graduate students. After his retirement from Kyoto University, he continued his educational work at Kyoto Sangyo University from 1981 to 1988 as a professor.

Dr. Takezaki has also made great contributions to the management and administration of ICR, Kyoto University, and other scientific communities. For example, he was director of ICR and member of the University Council, Kyoto University for two years from April 1974. He was director and adviser of Japan Petroleum Institute, and chairperson of JSMS Committee on High Pressure, The Society of Material Science, Japan.

His sincere and warm personality was respected by many friends, colleagues, students, and all those who came in contact with him. For his distinguished scientific achievements, he was honored with the Japan Petroleum Institute Award in 1976. In 1990, the Government made public recognition of his achievements by the Second Class of the Order of the Rising Sun, Gold and Silver Star, “Kun-Ni-Tou Kyoku-Jitsu-Shou” Medal.

Obituary

Professor Emeritus

Dr. TASHIRO, Megumi (1917–2008)

Dr. Megumi Tashiro, Professor Emeritus of Kyoto University, passed away on July 16, 2008, in Kyoto.

Dr. Megumi Tashiro was born in Tokyo on December 19, 1917. He graduated from Department of Ceramics, Tokyo Institute of Technology in 1940 and was enrolled in the Post-Graduate Course of Kyoto University (Industrial Chemistry Course) from May 1940 to September 1942. After two years and three months serving as Research Associate at Institute for Chemical Research (ICR), Kyoto University, he was promoted to Associate Professor of ICR in 1944. He was received Degree of Doctor of Engineering from Kyoto University in August 1949. He was also served as Visiting Associate Professor at Department of Mineral Industries, Pennsylvania State University (USA), from July 1953 to August 1956. In 1959, he was appointed Full Professor of ICR, Kyoto University to take charge of the Laboratory of Ceramic Chemistry. He was served as Director of ICR and the Member of the University Council, Kyoto University, from April 1978 to March 1980. He retired from Kyoto University and received Title of Professor Emeritus of Kyoto University in April 1981.

Dr. Tashiro made a significant contribution to the researches on (1) the porcelain enamel, (2) the preparation and properties of glasses, (3) the glass-ceramics and (4) the ceramics prepared by unidirectional solidification of melts. In the researches on the porcelain enamel, he elucidated the mechanism of adherence of enamel on steel surface, leading to the development of novel heat-resistant enamels. In the researches of optical glass, he established the homogenization of glass in tank furnace melting and succeeded in the improvement of the chemical durability of optical glass. The results of effects of high energy irradiation and high pressure on the properties of glass were widely appreciated. His most notable achievement is without doubt related to glass-ceramics. He found that the addition of ZrO_2 with P_2O_5 as the nucleating agents to the base glasses remarkably promoted the nucleation in the glasses, producing the glass-ceramics with high strength or high transparency depending on the heat-treatment condition. Based on the finding, a number of glass-ceramic wares have been commercialized by a Japanese glass company so far. These distinguished achievements in the respective fields are highly appreciated internationally as well as domestically. He was recipient of the Japanese Ceramic Association Award in 1953 for his research on enamels. Especially, he was honored with the Science Award from Kyoto News Paper in November 1963 and the Special Patent Award (the Award of the President of the Chamber Commerce and Industry, Japan) from the Patent Association of Japan in April 1967 for his significant achievement in the development of a new type of the glass-ceramics. He was honored with the Title of Fellow of the Society from the American Ceramic Society in April 1968.

Dr. Tashiro was a gentle and sincere man. He educated a lot of able students and young scientists. He served as the Regional Editor of the Journal of Non-Crystalline Solids from 1969 to 1981 and the Vice-President of the Ceramic Society of Japan. The Japanese Government made public recognition of his achievements by the Second Class of the Order of the Sacred Treasure, “Kun-Nitou Zuihoushou” medal in 2000 and granted the Grade of the Fourth Court Rank in 2008.

Obituary

Professor Emeritus

Dr. UYEDA, Natsu (1924–2008)

Dr. Natsu Uyeda, Professor Emeritus of Kyoto University, passed away unexpectedly on April 6, 2008, in Osaka.

Dr. Natsu Uyeda was born on October 4, 1924, in Kyoto. After graduating from Kyoto Imperial University in September, 1947, with his major in chemistry, he continued to study crystal chemistry under the supervision of the late Professor Emeritus Kenzo Tanaka at the Department of Physics, the Faculty of Science, Kyoto University. He was conferred the degree of Doctor of Science from Kyoto University for his studies on crystal structure analysis by using subsidiary maxima in electron diffraction in 1958.

Dr. Uyeda was appointed an Instructor at Institute for Chemical Research, Kyoto University in April, 1950, and started his academic career studying crystal and colloid chemistry in the laboratory of the late Professor Emeritus Eiji Suito. Dr. Uyeda was promoted to an Associate Professor in December, 1956 at the same institute. In March, 1976, he was appointed a Full Professor of the institute to direct the Laboratory of Crystal and Powder Chemistry until his retirement. He retired from Kyoto University on March 31, 1988 after 38 years service to the University, and was honored with the title of Professor Emeritus of Kyoto University on the next day.

Dr. Uyeda conducted extensive research in crystal chemistry. Specifically, his research fields included organic powdery crystal dispersion system, formation and structure of colloidal fine particles, organic thin film system, and high resolution electron microscopy. His pioneering achievements in these fields are highly appreciated internationally as well as domestically. The achievement, most widely recognized by the scientific community and very much cherished by himself, is the subject on high resolution imaging by electron microscopy using many beams synthesis method. In order to realize the world's first atomic imaging of molecules, he made huge contributions to introduce high voltage electron microscopes to Institute for Chemical Research.

Dr. Uyeda was invited to many international conferences to give special lectures on direct imaging of organic molecules in crystal using high resolution electron microscopy at atomic level. His stimulating presentations always attracted the interest of the audience. He was a member of many international organizing committees such as International Congress on Electron Microscopy and International Crystal Conference. For his high resolution electron microscopic study on thin films of organic semiconductors, Dr. Uyeda was awarded the Seto Prize from the Japanese Society of Electron Microscopy in 1964.

Dr. Uyeda gave lectures on crystal chemistry at the Graduate School of Science from 1961, and supervised the dissertation works of many talented graduate students. He authored and coauthored more than 150 scientific papers and several books, including the famous monograph, "The Achievement and Limitation of HV-HREM". Moreover, his beautiful molecular images by high resolution imaging were widely cited in many text books to stimulate young students in universities and high schools.

Owing to his sincere and warm personality, Dr. Uyeda won the respect and friendship of those who came in contact with him. In 2003, Japanese government made the public recognition of his achievements by the Order of the Sacred Treasure.

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

Mizuhata Y, Tokitoh N: (*E*)-*N*-{2-(9-Fluorenylidene)-3a,5,7-trimethyl-2*H*-indol-3-ylidene}-2,4,6-trimethylaniline, *Acta Cryst. E,* **64**, o493 (2008).

Nagahora N, Sasamori T, Hosoi Y, Furukawa Y, Tokitoh N: Generation, Isolation, and Reactivity of a Kinetically Stabilized Diphosphene Anion Radical, *J. Organomet. Chem.,* **693**, 625-632 (2008).

Matsumoto T, Sasamori T, Sato K, Takui T, Tokitoh N: Reduction of a Kinetically Stabilized Silabenzene Leading to the Formation of the Corresponding Anion Radical Species, *Organometallics,* **27**, 305-308 (2008).

Mizuhata Y, Tokitoh N: 9,9′-Dibromo-9,9′-bifluorene, *Acta Cryst. E,* **64**, o544 (2008).

Sasamori T, Tokitoh N: Doubly Bonded Systems between Heavier Group 15 Elements, *Dalton Trans.,*1395-1408 (2008).

Kajiwara T, Takeda N, Sasamori T, Tokitoh N: Synthesis of Alkali Metal Salts of Borylsilyl Anions Utilizing Highly Crowded Silylboranes and Their Properties, *Organometallics,* **27**, 880-893 (2008).

Isobe T, Mizuhata Y, Tokitoh N: Acyclic Tetrachalcogenoether Ligands Tethered with Bulky Substituents: Their Syntheses and Coordination Chemistry, *J. Organomet. Chem.,* **693**, 1225-1232 (2008).

Tokitoh N, Tajima T, Takeda N, Sasamori T: Synthesis and Characterization of the First Stable Stannanetellone, *Phosphorus, Sulfur, and Silicon and the Related Elements,* **183**, 948-955, (2008).

Sasamori T, Mieda E, Tsurusaki A, Nagahora N, Tokitoh N: Selenization and Tellurization Reactions of Kinetically Stabilized Dipnictenes, *Phosphorus, Sulfur, and Silicon and the Related Elements,* **183**, 998-1002 (2008).

Tanabe T, Mizuhata Y, Takeda N, Tokitoh N: Syntheses and Structures of Platinum Siloxides Bridged by a Sulfur or Selenium Atom and a Unique 1,3-Aryl Migration from Silicon to Platinum through the Si–O–Pt Linkages, *Organometallics,* **27**, 2156-2158 (2008).

Ozaki S, Sasamori T, Tokitoh N: Synthesis of a 1-Hydrosilene Stable in Solution and Its Unique Properties, *Organometallics,* **27**, 2163-2165 (2008).

Tanabe Y, Mizuhata Y, Tokitoh N: Mechanistic Investigation of the Hydration Reaction of [Cr(η^6-silabenzene)$(CO)_3$]: Hydrido-(silacyclohexadienyl)chromium Complex as an Intermediate, *Chem. Lett.,* **37**, 720-721 (2008).

Tokitoh N, Wakita K, Matsumoto T, Sasamori T, Okazaki R, Takagi N, Kimura M, Nagase S: The Chemistry of Stable Silabenzenes, *J. Chin. Chem. Soc.,* **55**, 487-507 (2008).

Sasamori T, Yuasa A, Hosoi Y, Furukawa Y, Tokitoh N: 1,2-Bisferrocenyldisilene: A Multi-step Redox System with an Si=Si Double Bond, *Organometallics,* **27**, 3325-3327 (2008).

Nagahora N, Sasamori T, Tokitoh N: Chalcogenation Reactions of a Stable Ferrocenyldiphosphene: Formation of Thia-, Selena-, and Telluradiphosphiranes, *Heteroatom Chem.,* **19**, 443-449 (2008).

Mizuhata Y, Sasamori T, Nagahora N, Watanabe Y, Furukawa Y, Tokitoh N: Synthesis and Properties of Stable 2-Metallanaphthalenes of Heavier Group 14 Elements, *Dalton Trans.,* 4409-4418 (2008).

Nagahora N, Sasamori T, Tokitoh N: A Ferrocenyldiphosphene-platinum Complex: Structural Features and Theoretical Calculations, *Organometallics,* **27**, 4265-4268 (2008).

Yamase K, Hayashi S, Nakanishi W, Sasamori T, Tokitoh N: Fine Structures of 1-(Arylethynylselanyl)naphthalenes: Characteristic Features Brought by the Ethynylselanyl Group, *Polyhedron,* **27**, 2478-2486 (2008).

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— Pathway Engineering —

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Takigawa I, Hashimoto K, Shiga M, Kanehisa M, Mamitsuka H: Efficiently Finding Significant Substructural Patterns Conserved in Glycans, *The Proceedings of the 2008 Annual Conference of the Japanese Society for Bioinformatics*, P066 (2008).

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INTERNATIONAL RESEARCH COLLABOLATIONS

[Australia]
Antarctic Climate and Ecosystems CRC, University of Tasmania

Caulfield School of Information Technology, Monash University

[Canada]
Department de Physique, Universite de Sherbrooke

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

Department of Mathematics, Fudan University

Department of Mathematics, Hong Kong Baptist University

Department of Mathematics, The University of Hong Kong

Department of Physics, National Taiwan University

Department of Polymer Science and Engineering, Shanghai Jiao Tong University

Institute of Physics, Chinese Academy of Science

Research Centre for Applied Sciences, Academia Sinica

[Finland]
Institute of Materials Chemistry Tampere, University of Technology

[France]
Bioinformatique Structurale, Institut Pasteur

Institut de Mineralogie et de Physique des Mileux Condenses, Universite Pierre et Marie Curie

Institute Laue Langevin

University of Rennes 1, Sciences Chimiques de Rennes

[Germany]
European Molecular Biology Laboratory

Max Planck Institute of Colloids and Interfaces

Max-Planck-Institut für Kernphysik

[Greece]
Department of Chemistry, University of Athens

Department of Materials Science & Technology, University of Crete

Institute of Electronic Structure & Laser, FORTH

[Italy]
Department of Genetics and Molecular biology, University of Rome “La Sapienza”

Dipartimento di Fisica, Università di Perugia

Dipartimento di Ingegneria Chimica, Universitȁ degli studi di Napoli “Federico II”

Institute of Biology and Agricultural Biotechnology (IBBA), National Research Council of Italy (CNR)

Istituto di Ricerche Sulla Combustione − CNR

University of Sassari, Laboratory of Science Material & Nano-technology, Alghero

[Korea, R.]
School of Chemical and Biological Engineering, Seoul National University

[Netherlands]
Swammerdam Institute for Life Science, University of Amsterdam

[Russia]
Joint Institute for Nuclear Research

[Sweden]
Department of Microbiology, Tumor and Cell Biology, Karolinska Institutet

Department of Physiological Chemistry II, Department of Medical Biochemistry and Biophysics, Karolinska Institute

Swedish Institute for Infectious Disease Control (SMI)

[Taiwan]
National Synchrotron Radiation Research Center

[UK]
Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh

ISIS Facility, Rutherford Appleton Laboratory

Welsh School of Pharmacy, Cardiff University

[USA]
CMPMS Department, Brookhaven National Laboratory

Department of Chemistry, University of Washington

Department of Molecular, Cellular & Developmental Biology, Yale University

Department of Oceanography, University of Hawaii

LASSP, Department of Physics, Cornell University

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

Section of Cell and Developmental Biology, University of California San Diego

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

THESES

ABE, Katsumasa
D Agr, Kyoto University
"Enzymatic Studies of Selenocysteyl-tRNA^{Sec} Biosynthesis"
Supervisor: Prof ESAKI, Nobuyoshi
23 January 2008

HAYASHI, Akito
D Eng, Kyoto University
"Studies of Late Transition Metal Complexes Bearing Phosphaalkene Ligands"
Supervisor: Prof OZAWA, Fumiyuki
24 March 2008

INOUE, Rintaro
D Eng, Kyoto University
"Dynamics in Polymer Thin Films by Inelastic Neutron Scattering"
Supervisor: Prof KANAYA, Toshiji
24 March 2008

ISOBE, Toru
D Sc, Kyoto University
"Synthesis of Polychalcogenoether Ligands Tethered with Bulky Substituents and Their Application to the Synthesis of Transition Metal Complexes"
Supervisor: Prof TOKITOH, Norihiro
24 March 2008

KAWAMOTO, Jun
D Agr, Kyoto University
"Studies of Cold-Adaptation Mechanism of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"
Supervisor: Prof ESAKI, Nobuyoshi
23 January 2008

KURAHASHI, Kensuke
D Sc, Kyoto University
"Studies on the Extraction Separation System Utilizing the Specific Complex Formation Reaction of Metal Ions with Macrocyclic Legands"
Supervisor: Assoc Prof UMETANI, Shigeo
24 March 2008

KUROKAWA, Suguru
D Agr, Kyoto University
"Biochemical Function of Mammalian Selenocysteine Lyase"
Supervisor: Prof ESAKI, Nobuyoshi
24 March 2008

MATSUMOTO, Takeshi
D Sc, Kyoto University
"Elucidation of Electrochemical Properties of Kinetically Stabilized Silaaromatic Compounds"
Supervisor: Prof TOKITOH, Norihiro
24 March 2008

MIYAKE, Ryoma
D Agr, Kyoto University
"Construction of a Protein Expression System by Using a Cold-adapted Bacterium, *Shewanella livingstonensis* Ac10, as a Host"
Supervisor: Prof ESAKI, Nobuyoshi
23 January 2008

MORIYAMA, Katsuhiko
D Pharm Sc, Kyoto University
"Metal Hydroxide-Promoted Asymmetric Alkylation via Memory of Chirality at Ambient Temperature"
Supervisor: Prof KAWABATA, Takeo
23 March 2008

MOROOKA, Saiko
D Sc, Kyoto University
"Kinetics and Path Selection of Aldehyde Disproportionations and Carbon-Carbon Bond Formation in Super- and Subcritical Water"
Supervisor: Prof NAKAHARA, Masaru
24 March 2008

MURAMATSU, Wataru
D Pharm Sc, Kyoto University
"Regioselective Acylation of Carbohydrates by Nucleophilic Catalysis"
Supervisor: Prof KAWABATA, Takeo
23 March 2008

NAGAHORA, Noriyoshi
D Sc, Kyoto University
"Studies on the Construction of Novel π-Conjugated Materials Utilizing Unique Properties of Diphosphene Compounds"
Supervisor: Prof TOKITOH, Norihiro
24 March 2008

NAKAGAWA, Yuichi
D Agr, Kyoto University
"Studies on Amide-Hydrolyzing Actvities of Pseudomonas aeruginosa Lipase by Directed Evolution"
Supervisor: Prof SAKATA, Kanzo and Assoc Prof HIRATAKE, Jun
23 January 2008

NAKATSUKA, Seiji
D Sc, Kyoto University
"Study on Physical Speciation of Trace Metals in Seawater and Their Interaction with Marine Ecosystem"
Supervisor: SOHRIN, Yoshiki
24 March 2008

OGAWA, Hiroki
D Eng, Kyoto University
"Phase Separation and Dewetting in Polymer Blend thin Films"
Supervisor: Prof KANAYA, Toshiji
24 September 2008

TAKAISHI, Kazuto
D Pharm Sc, Kyoto University
"Synthesis and Optical Properties of Axially Homochiral Oligonaphthalenes"
Supervisor: Prof KAWABATA, Takeo
23 March 2008

TAKEMOTO, Kazuhiro
D Inf, Kyoto University
"Analysis and Modeling of Biological Networks Based on Statistical Mechanics"
Supervisor: Prof AKUTSU, Tatsuya
24 March 2008

TAKEUCHI, Toshihide
D Pharm Sc, Kyoto University
"Direct Translocation of Arginine-Rich Peptides through Plasma Membranes into Cells"
Supervisor: Prof FUTAKI, Shiroh
24 March 2008

TANABE, Mikio
D Sc, Kyoto University
"Longitudinal and Transverse Coupling of the Beam Temperature Caused by the Laser Cooling of $^{24}Mg^{+}$"
Supervisor: Prof NODA, Akira
24 March 2008

YAN, Wei
D Pharm Sc, Kyoto University
"Design of Artificial 6-Zinc Finger Peptides: Linker Alteration and DNA Binding Specificity"
Supervisor: Prof FUTAKI, Shiroh
24 March 2008

YOSHIDA, Ken
D Sc, Kyoto University
"Translational Dynamics in Supercritical Water Studied by High-Temperature NMR and Molecular Dynamics Simulation"
Supervisor: Prof NAKAHARA, Masaru
24 March 2008

THE 108TH ICR ANNUAL SYMPOSIUM

SEMINARS

MEETINGS AND SYMPOSIA

THE 108TH ICR ANNUAL SYMPOSIUM

(5 December 2008)

ORAL PRESENTATIONS

IKENOUCHI, Junichi (Supramolecular Biology)
"Elucidation of Molecular Mechanisms which Generate and Maintain Discrete Membrane Domains in Polarized Cells"

AKUTSU, Tatsuya (Biological Information Networks)
"Kernel-based Approaches to Classification and Design of Chemical Compounds"

MIZUHATA, Yoshiyuki (Organoelement Chemistry)
"The Chemistry of 'Heavy Aromtics'"

MURATA, Yasujiro (Structural Organic Chemistry)
"Synthesis and Properties of Open-Cage Fullerenes and Endohedral Fullerenes"

YOSHIMURA, Tomoyuki, et al. (Synthetic Organic Chemistry)
"Asymmetric Synthesis via Planar Chiral Enolates"

KURATA, Hiroki, et al. (Electron Microscopy and Crystal Chemistry)
"Development of a Scanning Transmission Electron Microscope Equipped with a Nanotip-FEG and Its Application to Local Analysis"

SAITO, Takashi (Advanced Solid State Chemistry)
"Synthesis and Physical Properties of the A-site-ordered Perovskites $AA'_3B_4O_{12}$"

TAKITA, Ryo (Organotransition Metal Chemistry)
"Synthesis and Properties of All-cis Poly(arylene vinylene)s Containing Thiophene Cores"

– ICR Award for Young Scientists –
GOTO, Atsushi (Chemistry of Polymer Materials)
"Reversible Chain Transfer Catalyzed Polymerization(RTCP): A New Class of Living Radical Polymerization"

– ICR Award for Graduate Students –
HARUTA, Mitsutaka (Electron Microscopy and Crystal Chemistry)
"Atomic Resolution ADF-STEM Imaging of Organic Molecular Crystal of Halogenated Copper Phthalocyanine"

MATSUNAGA, Ryusuke (Photonic Elements Science)
"Evidence for Dark Excitons in a Single Carbon Nanotube due to the Aharonov-Bohm Effect"

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

LW "Synthesis and Properties of Novel Organic Compounds Containing Hevier Elements"

GE TSURUSAKI, Akihiro; SASAMORI, Takahiro; TOKITOH, Norihiro
"Cycloaddition Reactions of an Overcrowded 9-Anthryldiphosphene"

GE MATSUMOTO, Teruyuki; SASAMORI, Takahiro; TOKITOH, Norihiro
"Design and Syntheses of a Novel Iminophosphido Ligand and Its Complexation Reactions"

GE INAMURA, Koji; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
"Structures and Reactivity of 9-Sila- and 9-Germaphenanthrene Complexes"

GE TANABE, Yusuke; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
"Elucidation of the Hydration Mechanism of Silabenzene-$Cr(CO)_3$ Complex and the Chemistry of Related Compounds"

— Structural Organic Chemistry —

LW "Synthesis of Endohedral Fullerenes by Means of Organic Synthesis and Their Properties"

GE KUROTOBI, Kei; MURATA, Michihisa; MURATA, Yasujiro
"Synthesis and Properties of Open-Cage Fullerene with Expanded π-Conjugated System"

— Synthetic Organic Chemistry —

LT HAYASHI, Kazuhiro; CHANGSHENG, Jiang; YOSHIMURA, Tomoyuki; TSUBAKI, Kazunori; SASAMORI, Takahiro; TOKITOH, Norihiro; KAWABATA, Takeo
"Synthesis and Properties of Novel Axially Chiral Binaphthyls Consisting of N-H-N Hydrogen Bond"

GE WATANABE, Toshihide; KAWABATA, Takeo
"Asymmetric Aldol Reactions via Memory of Chirality"

— Chemistry of Polymer Materials —

LT KYO, Shogyo; KAYAMA, Yuzo; ARITA, Toshihiko; OHNO, Kohji; FUKUDA, Takeshi; TSUJII, Yoshinobu
"Synthesis of Thick, Concentrated Polymer Brushes by High-pressure LRP"

GE AKASHI, Tatsuki; OHNO, Kohji; FUKUDA, Takeshi; TSUJII, Yoshinobu
"Surface-Initiated Atom Transfer Radical Polymerization on Narrowly Size-Distributed Silica Nanoparticles of Diameters less than 100 nm"

— Polymer Controlled Synthesis —

GE UKAI, Yu; MATSUMOTO, Atsushi; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
"Photo Induced Living Radical Polymerization Using Organotellurium Compounds"

GE YAMADA, Hiroto; KAYAHARA, Eiichi; YAMAGO, Shigeru
"Synthesis of End-Functionalized Polymers through Heavier Heteroatom-Metal Exchange Reactions"

GE UEKI, Kazuya; YAMAGO, Shigeru
"Synthesis of Oligo(Aromatic Ketone)s by Iterative Friedel-Crafts Reaction"

— Inorganic Photonics Materials —

LT OKU, Satoshi; TOKUDA, Yomei; TAKAHASHI, Masahide; YOKO, Toshinobu
"Novel Solvent-free Synthesis of Proton-conducting Organic-inorganic Hybrid Materials"

LT OKA, Takanori; TOKUDA, Youmei; TAKAHASHI, Masahide; YOKO, Toshinobu
"Quantitative Analysis for Quadrupolar Nuclei in Amorphous Materials"

LT MIYAGAWA, Yuya; TAKAHASHI, Masahide; TOKUDA, Youmei; YOKO, Toshinobu
"Organo-silico-phosphate Photosensitive Film for Active Microoptics"

— Nanospintronics —

GE NAKANO, Kunihiro; NAKATANI, Yoshinobu; OSHIMA, Norikazu; KASAI, Shinya; KOBAYASHI, Kensuke; ONO, Teruo
"Real-time Detection of the Current Induced Vortex Dynamics by using the TMR Effect"

GE YAMAUCHI, Yoshiaki; HASHISAKA, Masayuki; NAKAMURA, Shuji; KASAI, Shinya; KOBAYASHI, Kensuke; ONO, Teruo
"Measurement of the Shot Noise in a Quantum Dot"

— Biofunctional Design-Chemistry —

LW "Progress in Biofunctional Design Chemistry"

GE NAKAMURA, Atsushi; IMANISHI, Miki; FUTAKI, Shiroh
"Control of a Circadian Clock Gene by Artificial Zinc-finger Type Transcription Factors"

— Chemistry of Molecular Biocatalysts —

LW "Research Activities of Laboratory of Chemistry of Molecular Biocatalysts"

GE IKEUCHI, Hideyuki
"Inhibitors of Asparagine Synthetase -Molecular Design and Synthesis-"

— Molecular Biology —

LT TANIGUCHI, Y. Yukimi; TSUGE, Tomohiko; AOYAMA, Takashi
"Role of the Arabidopsis Phospholipase D Gene PLDζ2 under Phosphate-starved Conditions"

— Chemical Biology —

LW Chemical Biology

GE YAMAZOE, Sayumi; SHIMOGAWA, Hiroki; SATO, Shin-ichi; UESUGI, Motonari
"Discovery of Adhesamine, a Dumbbell-shaped Small Molecule that Promotes Cell Adhesion"

— Molecular Materials Chemistry —

GE SHIMAHARA, Yurie; KIMURA, Hironobu; FUKUSHIMA, Tatsuya; OYAMADA, Takahito; ENDO, Ayataka; YAHIRO, Masayuki; ADACHI, Chihaya; KAJI, Hironori
"Effect of Dynamics on Photoluminescence of Tetraphenyl-pyrene (TPPy), a Material for Organic Light-Emitting FETs"

GE FUKUSHIMA, Tatsuya; TAKAMI, Kousuke; KAJI, Hironori
"Organic Light Emitting Diodes Fabricated from Alq_3 in Different Crystalline Polymorphs"

GE TAKAMI, Kosuke; YAMADA, Tomonori; KAJI, Hironori
"Crystal Structure Analysis of *N,N'*-diphenyl-*N,N'*-di(*m*-tolyl) benzidine (TPD) by Two-Dimensional Double-Quantum Solid-State NMR"

GE YAMADA, Tomonori; KAJI, Hironori
"Percolation Paths for Charge Transports in TPD, a Hole-transport Material for Organic Light-emitting Diodes"

— Hydrospheric Environment Analytical Chemistry —

LW "Recent Topics from Hydrospheric Environment Analytical Chemistry"

GE OKABE, Taro; TANIGAWA, Masahito; UMETANI, Shigeo; SOHRIN, Yoshiki
"Ion Imprinted Sol-gel Materials for the Separation of Metal Ions"

— Solution and Interface Chemistry —

LT SHINTANI, Megumi; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru
"NMR Analysis of the Delivered Drugs in the Phospholipid Bilayer Membrane"

GE KIMURA, Hiroshi; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru
"NMR Analysis of Pyrolytic Behaviors of Saccharides"

— Molecular Microbial Science —

LT OMORI, Taketo; HONDA, Ai; MIHARA, Hisaaki; KURIHARA, Tatsuo; ESAKI, Nobuyoshi
"Novel Biological Phospholipids"

GE MOWAFY, Amr; KURIHARA, Tatsuo; MIHARA, Hisaaki; ESAKI, Nobuyoshi
"2-Haloacrylate Dehalogenase, a Novel Enzyme Representing a New Class of Hydratases"

— Polymer Materials Science —

LW "Recent Research for Polymer Materials Science Laboratory"

GE TANAKA, Kentaro; NISHIDA, Koji; KANAYA, Toshiji
"Critical Dissolution Ionic Strength of Aqueous Solution of Chitosan"

— Molecular Rheology —

GE CHEN, Quan
"Component Dynamics in Polyisoprene/Poly(4-tert-butylstyrene) Miscible Blends"

GE MISHIMA, Eri; YAMADA, Takeshi; YAMAGO, Shigeru; WATANABE, Hiroshi
"Development of Living Cationic Polymerization using Organotellurium Compounds"

GE TANAKA, Satoshi
"Dynamics of Star-block Copolymer during Elasticity Recovery after Cessation of Flow"

GE SUZUKI, Takeshi
"SCF Caluculation of Conformation of Polymer Chain for Multiblock Copolymers"

— Molecular Aggregation Analysis —

LT YOSHIDA, Hiroyuki; WATAZU,Yuji; MURDEY, Richard; SATO, Naoki
"Structure and Molecular Orientation in Vacuum-Deposited Thin Film of Bis(benzo)pentathienoacene"

GE HIRAMATSU, Takaaki; YOSHIDA, Hiroyuki; SATO, Naoki
"Structural Features of Polymorphic Crystalline Transition of an Amphoteric and Polar Molecule: BMDCM"

GE UCHINO, Yosuke; YOSHIDA, Hiroyuki; MURDEY, Richard; SATO, Naoki
"Frontier Electronic Structure in an Evaporated Thin Film of Bis(catecholate)diboron"

— Supramolecular Biology —

LT KUBO, Akira
"Identification and Fuctional Analysis of Lipids Constituing Cell-surface Membrane"

LT SUZUKI, Harumitsu; KATO,Utako; UMEDA,Masato
"A Role for Fatty Acid Desaturase in Energy Metabolism"

— Particle Beam Science —

GE YAMADA, Masako
"Development of Permanent Magnet Sextupole for Pulsed Cold Neutron Beam"

GE NAKAO, Masao; SOUDA, Hikaru; WAKITA, Akihisa; TONGU, Hiromu; NODA, Akira; TANABE, Mikio; ISHIKAWA, Takehiro; IKEGAMI, Masahiro; SHIRAI, Toshiyuki
"Two Dimensional Laser Cooling at S-LSR"

— Laser Matter Interaction Science —

LW "Advances in Laser Matter Interaction Science"

GE NAMBA, Shin; HASHIDA, Masaki; OKAMURO, Kiminori; TOKITA, Shigeki; SAKABE, Shuji
"Mechanism of Nano-ablation for Metals with Femtosecond Laser"

GE MASUNO, Shin-ichiro; TOKITA, Shigeki; HASHIDA, Masaki; SAKABE, Shuji
"Formation of Isolated Minute Thin Films by Laser Induced forward Transfer"

— Structural Molecular Biology —

GE ITO, Yoshiaki; TOCHIO, Tatsunori; HANDA, Katsumi; OOHASHI, Hirofumi; FUKUSHIMA, Sei; BLAICU, Aurel; TERASAWA, Mititaka
"Chemical States Obtained using a High-resolution Double-crystal X-ray Fluorescence Spectrometer"

LW "Recent Research Topics in Laboratory of Structural Molecular Biology"

GE ITO, Yoshiaki; SHIGEOKA, Nobuyuki; TOCHIO, Tatsunori; OOHASHI, Hirofumi; YOSHIKAWA, Hideki; FUKUSHIMA, Sei
"Evaluation of the Absorption Edge from the Evolution Spectra"

— Organic Main Group Chemistry —

LW "Recent Research Topics from Organic Main Group Chemistry"

GE NAKAGAWA, Naohisa; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
"Iron-Catalyzed Cross-Coupling Reaction between Alkenylzinc Reagents and Alkyl Halides"

GE TAKAYA, Hikaru; ISOZAKI, Katsuhiro; HAGA, Yusuke; FUKUI, Sadayuki; SASANO, Daisuke; SEIKE, Hirofumi; NAOTA, Takeshi; NAKAMURA, Masaharu
"Metallated Peptides: Synthesis, Structure, and Functions"

GE YOSHIMOTO, Yuya; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
"Iron-Catalyzed Enyne Cross-Coupling Reaction"

GE ITOH, Takuma; ITO, Shingo; NAKAMURA, Eiichi; NAKAMURA, Masaharu
"Iron-Catalyzed Enantioselective Carbometalation of Oxabicyclic Alkenes with Aryl Zinc Reagents"

— Advanced Solid State Chemistry —

LT SAITO, Takashi
"Magnetism of the A-site-ordered Perovskite $CaCu_3(Ge, Ti,Sn)_4O_{12}$"

LW "Recent Research Topics of Laboratory of Advanced Solid State Chemistry"

GE INOUE, Satoru; KAWAI, Masanori; SHIMAKAWA, Yuichi
"Epitaxial Thin Films of $SrFeO_2$ with FeO_2 Infinite Layers by CaH_2 Low Temperature Reduction"

GE LONG, Youwen
"High Pressure Synthesis and Intermetallic Charge Transfer in $LaCu_3Fe_4O_{12}$ Double Perovskite"

— Organotransition Metal Chemistry —

LW "Activity Report: Organotransition Metal Chemistry Laboratory"

GE NAKAJIMA, Yumiko; OZAWA, Fumiyuki
"Synthesis and Property of Transition Metal Complexes Bearing a Phosphaalkene Ligand"

— Bioknowledge Systems —

LW "KEGG Database and GenomeNet Pharmaceutical Products Database"

— Biological Information Networks —

GE POOLSAP, Unyanee
"Prediction of RNA Secondary Structure with Pseudoknots Using Integer Programming"

— Pathway Engineering —

LT HASHIMOTO, Kosuke; TAKIGAWA, Ichigaku
"Efficiently Finding Significant Substructural Patterns Conserved in Glycans"

— Research Center for Low Temperature and Materials Sciences —

LT TERASHIMA, Takahito; NII, Akinori; SHISHIDO, Hiroaki; YASU, Kazuki; KATOU, Tomonari; SHIBAUCHI, Takasada; MATSUDA, Yuji
"Preparation and Transport Properties of Heavy-Fermion Superlattices"

SEMINARS

Dr ARGYRIOU, Dimitr
Helmholtz Zentrum Berlin, Germany
"Strong Spin-Lattice Coupling in Layered $CaFe_2As_2$ and PrFeAsO"
22 August 2008

Prof ARNOLD, John
College of Chemistry, University of California, Berkeley, USA
"Olefin Polymerization with Early Transition Metal Catalysts"
12 February 2008

Prof CHAMOVITZ, A Daniel
Department of Plant Sciences, Tel Aviv University, Israel
"Genomic Analysis of the COP9 Signalosome–Lessons From *Drosophila*, Implications for *Arabidopsis*"
10 November 2008

Mr CHRISTFOROS, Moutafis
Cavendish Laboratory, Cambridge University, Cambridge, UK
"Statics and Dynamics of Bubble Domains in Nanodots with High Anisotropy"
3 June 2008

Prof CRUDDEN, Cathleen
Queen's University, Kingston, Canada
"Catalysis and Chirality with Molecules and Materials"
20 May 2008

Dr DOHMAE, Naoshi
Biomolecular Characterization Team, Wako Institute, RIKEN, Saitama, Japan
"Detailed Structural Analyses on Proteins"
17 January 2008

Dr FLÖRSHEIMER, Mathias
Research Centre Karlsruhe, Institute for Nuclear Waste Deposition, Germany
"Speciation and Hydration of Mineral Surfaces Determined at the Molecular Level"
5 June 2008

Prof FUJIKAWA, Seizo
Department of Agriculture, Hokkaido University, Hokkaido, Japan
"Non-Freezable Water"
19 December 2008

Prof GABRYS, Barbara J
Department of Materials Science, University of Oxford, UK
"SANS and Wide Angle Scattering from Model Bulk Ionomers"
13 May 2008.

Prof GRIESER, Manfred
Max Planck Institute, Germany
"Recent Developments at the Storage Ring TSR and the Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics"
21 November 2008

Prof HANDA, Sandeep
University of Leicester, Leicester, UK
"The Synthesis of Biologically Active Nitrogen Heterocycles"
11 March 2008

Vis Prof HORIMOTO, Katsuhisa
Computational Biology Research Center, Advanced Industrial Science and Technology, Tokyo, Japan
"Analysis of Dynamics of Biological Networks Using Symbolic Computation"
20 May 2008

Prof HVILSTED, Søren
Technical University of Denmark, Lyngby, Denmark
"Novel Polymer Architectures for Optical Storage by Holography"
10 November 2008

Ms IAFRATE, Silvia
Institute of Biology and Agricultural Biotechnology, National Research Council of Italy, Italy
"Roles of Class I KNOX Transcription Factors in Gene Regulation During Shoot Development of *Arabidopsis thaliana*"
6 November 2008

Prof IWATA, Hiroo
Institute for Frontier Medical Sciences, Kyoto University, Japan
"Reparative Materials for Polymer Gel"
24 June 2008

Prof JAMESON, Robert A
Goethe University, Germany
"Discussion on Comparison of Design and Simulation Codes for RFQs"
9 May 2008

Dr KAMIKAWA, Takashi
Sumitomo Chemical Co. Ltd.
"Development of Cross-coupling Reaction Using Nickel Catalysts"
5 May 2008

Prof KATO, Takeo
Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan
"Thermal Transport in Quantum Dots"
4 November 2008

Prof KIM, Byeang Hyean
Pohang University of Science and Technology, Pohang, Korea
"Modified Nucleic Acid Systems for Biomedical Applications"
10 November 2008

Prof KITAOKA, Takuya
Department of Agriculture, Kyushu University Fukuoka, Japan
"Material Chemistry of Functional Polysaccharides"
18 December 2008

Prof KOTORA, Martin
Department of Organic and Nuclear Chemistry, and Centre for New Antivirals and Antineoplastics, Faculty of Science, Charles University, Czech Republic
"Synthesis of Estrone Based on Organometallic Reactions"
4 August 2008

Prof KÜNDIG, E Peter
Department of Chemistry, University of Geneva, Switzerland
"New Ligand and Transition Metal Catalysts for Asymmetric Synthesis"
29 May 2008

Prof LEE, Jae-Suk
Gwangju Institute of Science and Technology, Gwangju, Korea
"Living Anionic Polymerization of n-Hexyl Isocyanate"
31 January 2008

Prof LOH, Tech Peng
Nanyang Technological University, Singapore
"In Search of New Methods and Concepts in Organic Synthesis"
11 December 2008

Prof MARRUCCI, Giuseppe
Universita degli Studi di Napoli "Federico II"
"Constitutive Modeling of Nonlinear Rheology"
21 March 2008

Prof MATSUNO, Kenji
Faculty of Industrial Science and Technology, Tokyo University of Science, Tokyo, Japan
"Mechanisms of Left-right Asymmetry Determination in *Drosophilla*—Genetical and Computational Approach—"
17 March 2008

Dr MENON, Suchithra
Molecular, Cellular, and Developmental Biology, Yale University, USA
"Functions of COP9 Signalosome Subunit 8 (Csn8) in Mammalian Development and T cell Immune Responses"
10 January 2008

Dr MIURA, Takashi
Graduate School of Medicine, Kyoto University, Kyoto, Japan
"How Morphogenesis in Development can Be Understood by Computation?"
29 January 2008

Dr MIYATAKE, Hideyuki
Biomolecular Characterization Team, Wako Institute, RIKEN, Saitama, Japan
"Introduction to the Technical Achievements on Crystallization of Proteins and X-ray Diffraction Analyses"
17 January 2008

Prof MOROKUMA, Keiji
Fukui Memorial Research Institute, Kyoto University, Japan
"Recent Advances in Computational Chemistry in Nano Science"
9 December 2008

Prof MUKHERJEE, Manabendra
Surface Physics Division, Saha Institute of Nuclear Physics, India
"Neutralization Kinetics of Charged Polymer Surfaces: A Photoemission Study."
27 March 2008

Prof NORIKI, Shinichiro
Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan
"Elemental Cycling based on the Settling Particles — the Western Pacific and the Japan Sea"
5 December 2008

Prof PROCHIANTZ, Alain
Ecole Normale Supérieure/Collège de France
"Protein Transduction: a Novel Physiological Signaling Mechanism and a Tool in Therapeutic Studies"
25 September 2008

Assoc Prof RYSZARD, Ostaszewski
Polish Academy of Science, Warszawa, Poland
"Enzymes in Stereoselective Synthesis of Biologically Active Compounds"
21 January 2008

Prof SAITO, Takafumi
Tokyo University of Agriculture and Technology, Tokyo, Japan
"Compact Visualization of Large Scale Data"
25 July 2008

Dr dos SANTOS, Antonio Moreira
Oak Ridge National Laboratory
"High-Pressure Studies of Crystalline and Amorphous Ge Based Clathrates"
22 August 2008

Prof SCHIEBER, Jay
Illinois Institute of Technology
"Molecular Modeling and Linear Viscoelasticity"
21 March 2008

Prof SCHWECHHEIMER, Claus
Department of Plant Systems Biology, Technical University of Munich, Germany
"A Novel Auxin Transport Regulatory Protein Kinase from *Arabidopsis thaliana*"
10 November 2008

Prof SERINO, Giovanna
Department of Genetics and Molecular Biology, University of Rome "La Sapienza", Italy
"Regulation by the COP9 Signalosome of AtPIC2, an F-box Protein from *Arabidopsis thaliana*"
6 November 2008

Prof SHIMIZU, Hirohiko
Institute of Materials Structure Science, High Energy Accelerator Research Organization, Japan
"Recent Trend in Neutron Source Development and Applications"
10 October 2008

Prof SUZUKI, Akemi
Future Science and Technology Joint Research Center, Tokai University, Tokyo, Japan
"Tissue Specific Distribution of Glycolipids"
19 March 2008

Prof SUZUKI, Akira
Hokkaido University, Japan
"Organic Synthesis using Organoborane Compounds"
21 November 2008

Prof TILSET, Mats
Department of Chemistry, University of Oslo, Norway
"Mechanisms of Hydrocarbon C-H Activation at Pt(II) Complexes"
29 February 2008

Assoc Prof TSAI, Francis T F
Baylor College of Medicine, Houston, Texas, USA
"Visualizing the Structure of a Molecular Machine"
11 November 2008

Prof TSUJI, Hideto
Department of Ecological Engineering, Toyohashi University of Technology, Japan
"High Performance Material for Poly(lactic acid) Stereo Complex"
3 July 2008

Prof QU, Li-Jia
College of Life Sciences, Peking University, China
"Molecular Mechanism of the Curly Leaf Phenotype in the Rice Curly-Flag-Leaf Mutant *cfl1*"
7 August 2008

Prof WATANABE, Junji
Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, Japan
"Crystals of Polypeptides"
4 April 2008

Dr WIENGMOON, Amporn
Naresuan University, Thailand
"The Use of Electron Microscopy for the Microstructural Characterization of High Chromium Cast Irons"
31 Octorber 2008

Prof WOODWARD, Patrick
Ohio State University, USA
"Cation and Anion Ordering in Complex Perovskites"
27 August 2008

Prof WIRTH, Thomas
Department of Chemistry, Cardiff University, Cardiff, UK
"New Concepts for Catalysis in Modern Synthesis"
26 September 2008

Dr YAMADA, Yoichi M. A.
Emergent Materials Department, Advanced Science Institute, RIKEN, Japan
"Development of Polymeric Complex Catalysts via Molecular Convolution"
6 November 2008

Prof YAMANAKA, Masahiro
Department of Chemistry, College of Science, Rikkyo University, Japan
"Catalyst Development and Ligand Design Based on Quantum Chemical Calculation"
21 November 2008

Mr YANN, Le Maho
Universit Paris-Sud, Orsay France
"Contributions of Spin Waves to Domain Wall Dynamics"
22 May 2008

Prof YAN, Shouke
Institute of Chemistry, Chinese Academy of Sciences, China
"Orientation Induced Crystallization of iPP–the Origin of Beta Crystallization"
16 May 2008

Prof ZIPSE, Hendrik
Ludwig-Maximilians-Universität in München, München, Germany
"Benchmarking Organocatalytic Processes"
9 September 2008

MEETINGS AND SYMPOSIA

The Sixth Asia Pacific Bioinformatics Conference (APBC2008)
Organized by AKUTSU, Tatsuya
14–17 January 2008 (Kyoto, Japan)

The Third International Workshop for Far East Asian Young Rheologists
Co-organized by ICR, Seoul National University, and Shanghai Jiao Tong University
25–27 January 2008 (Shanghai, China)

The 64th Annual Meeting of the Japanese Society of Microscopy (JSM 2008)
Organized by ISODA, Seiji
21–23 May 2008 (Kyoto, Japan)

The 2nd International Symposium on Synergy of Elements "International Symposium on Chemistry of Concerto Catalysis Based on Synergy of Elements"
Organized by OZAWA, Fumiyuki
12 July 2008 (Rennes, France)

The 41st Summer Seminar for Young Peptide Scientist
Organized by NAKASE, Ikuhiko; YANO, Yoshiaki
3–5 August 2008 (Kyoto, Japan)

The 3rd International Symposium on Synergy of Elements "2008 Workshop on Organometallic Chemistry"
Organized by OZAWA, Fumiyuki
9 October 2008 (Beijing, China)

The 2nd Mini Peptide Symposium for Young Researchers
Organized by NAKASE, Ikuhiko; YANO, Yoshiaki
28 October 2008 (Tokyo, Japan)

The 3rd Taiwan-Japan Workshop on Neutron Scattering of Bio-materials and Soft-matters for Nanotechnology and Biotechnology
Organized by KANAYA, Toshiji
4–6 December 2008 (Kyoto, Japan)

BMB2008 (The 31th Annual Meeting of MBSJ & the 81th Annual Meeting of JBS) "Lipid Biology of Model Organisms"
Organized by UMEDA, Masato
9–12 December 2008 (Kobe, Japan)

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Institute for
Chemical
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