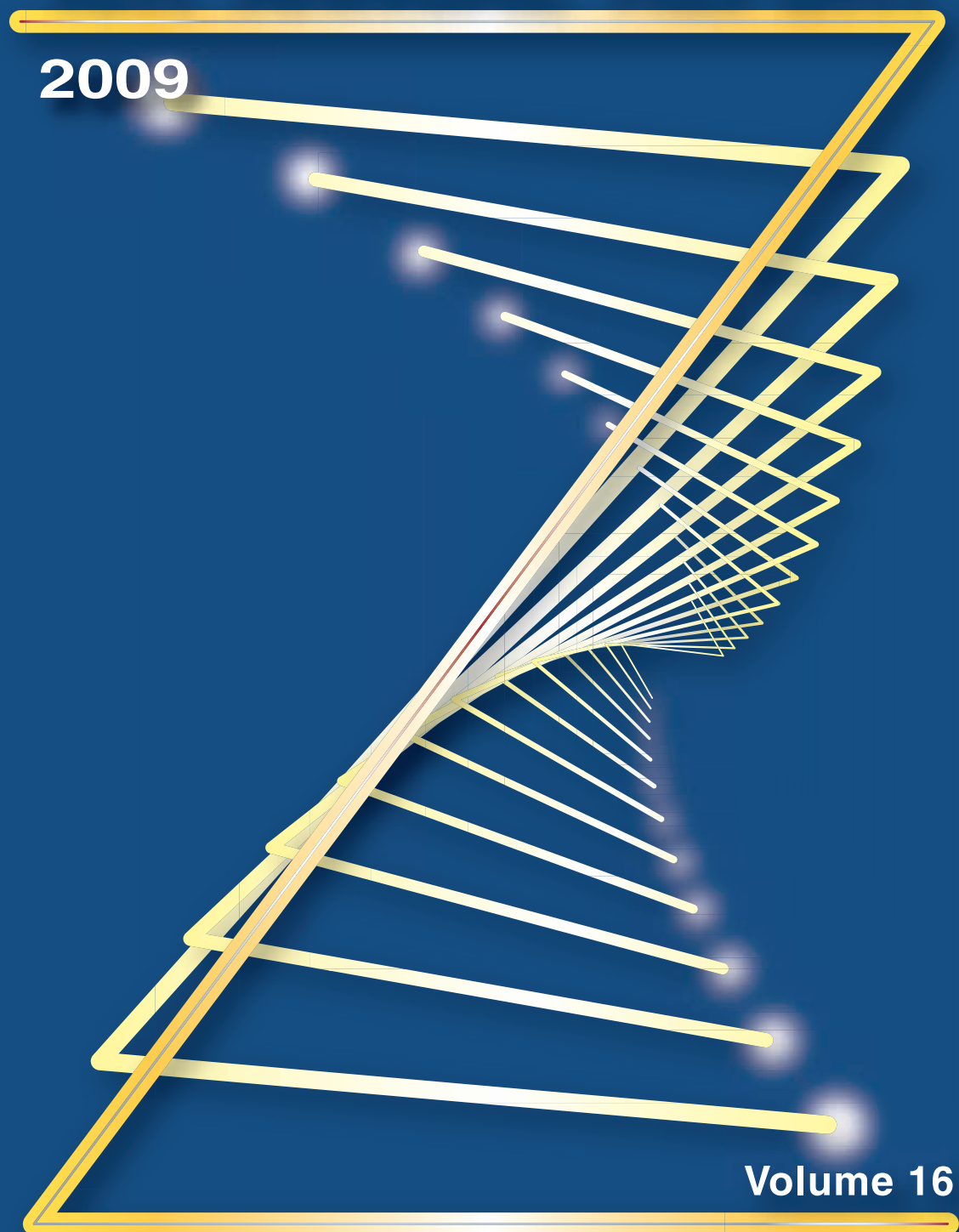


ICR ANNUAL REPORT

2009



Volume 16

Institute for Chemical Research
Kyoto University

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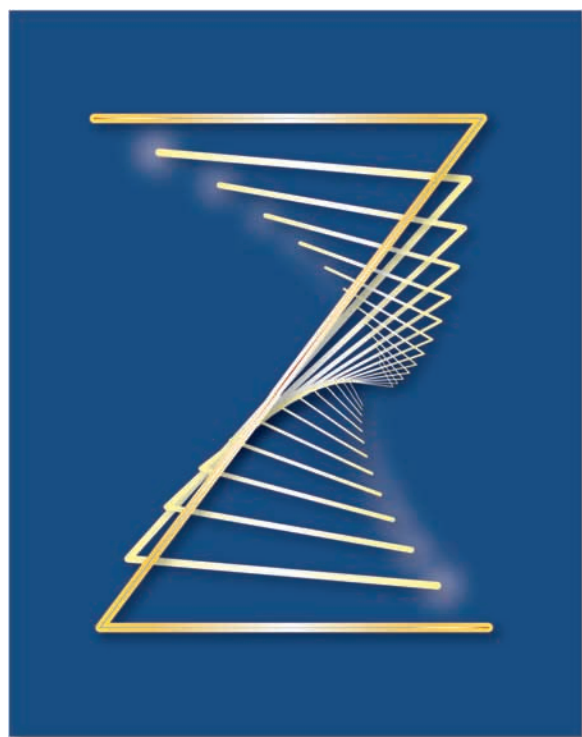
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**ICR
ANNUAL
REPORT
2009**



**Institute for Chemical Research
Kyoto University**
Volume 16



Preface

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 its 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 further to promote research collaborations, which are not easy in conventional graduate schools. Moreover, we aim to utilize our strengths as an outstanding center in education in order to produce excellent scientists and engineers who can actively contribute to our global society on the basis of their broad and profound perspective.

ICR is currently executing Global COE Programs in collaboration with the Graduate School of Engineering and the Graduate School of Science. These Programs include “International Center for Integrated Research and Advanced Education in Material Science (starting from 2007)” encompassing chemistry and materials science fields, “Center of Excellence for Education and Research on Photonics and Electronics Science and Engineering (from 2007)” involving information science, electrical engineering, and electronics fields, and “The Next Generation of Physics, Spun from University & Emergence Developing Independent Researchers to Explore New Frontiers (from 2008)” covering physics, astronomy, and materials chemistry fields. In addition, ICR is making enthusiastic contribution to the “Joint Project of Chemical Synthesis Core Research Institutions (2005-2010)”, 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. Furthermore, ICR is currently collaborating with domestic/oversea universities and research organizations (with 43 official international collaboration agreements) and is going to function as a Joint Usage/Research Center supported by MEXT (since 2010).

The strong collaboration basis so far constructed in-house and also with outside ensures our institute to serve as the core of global research propellers in chemistry-oriented fields. Thus, we respectfully request your continued support and encouragement.

January 2010

TOKITOH, Norihiro
Director

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 produced 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 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 113 faculty members and about 230 graduate students. Each laboratory belongs to one of the seven graduate schools which encompass science, engineering, pharmaceutical science,

ICR News 2009

ICR Activity as the Joint Usage/Research Center (JURC)

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



1	3	5	7
2	4	6	8

1. Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry (MALDI-TOFMS)
2. Ion Storage/Cooler Ring, S-LSR
3. Intense Short-Pulse Laser System
4. GenomeNet Server
5. High Resolution Electron Spectromicroscope
6. High Resolution Magnetic Sector Field Inductively Coupled Plasma Mass Spectrometry
7. Angle-Resolved Photoemission Spectrometer
8. 800MHz Nuclear Magnetic Resonance Spectrometer

Institute for Chemical Research (ICR) has been approved by MEXT Japan as the “Joint Usage/Research Center (JURC)” for development and cooperation in chemistry-oriented research fields and will fully function as JURC from 2010. The ICR has been conducting frontier research in a wide range of chemistry-oriented fields that include particle/quantum beam science, organic/inorganic/polymeric materials science, biological science, and bioinformatics. On the basis of the significant width and depth of the research activities at ICR as well as the obvious domestic/international collaboration achievements of ICR supported by more than 40 memoranda of agreement, JURC invites the researchers outside of ICR to collaborate closely with the ICR faculty members (all concurrently belonging to JURC) and also to jointly utilize the precise/powerful/extensive instruments/facilities/databases equipped at ICR (cf., photos shown above).

Reflecting the opinions and/or requests from the researchers outside of ICR, JURC will carry out frontier and/or interdisciplinary joint research categorized in the following four classes: specific subjects chosen by JURC such as “creation of novel materials and survey of their functionalities based on elements science”, on-demand

subjects from the researchers outside of ICR, interdisciplinary subjects emphasizing development of new collaboration such as “set-up of an inter-university joint research team focusing on interdisciplinary aspects of materials analysis”, and subjects focusing on the joint usage of JURC/ICR facilities such as the ultra-high resolution solid state NMR. This activity of JURC is based on a newly founded “Collaborative Research Station” that consists of open laboratories for both in-house and external researchers involved in the JURC joint research program, research divisions of visiting professors, a management office maintaining the instruments/facilities/databases for the joint use, and the headquarters supporting both administrative and technical aspects of the joint research.

The joint research activities mentioned above ensure that JURC/ICR will serve as the core force of global research in chemistry-oriented fields and train young researchers who will sustain and develop these fields in the near future. JURC/ICR cordially invites warm and friendly support from researchers and communities in chemistry-oriented fields of science.

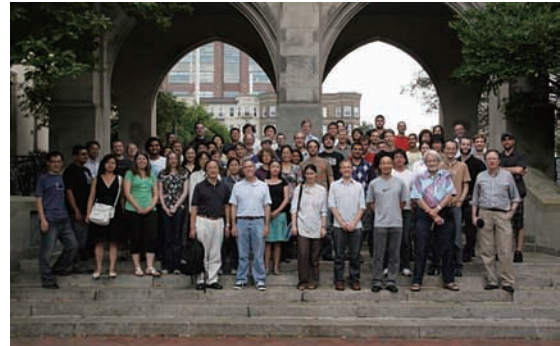
International Research and Training Program on Bioinformatics and Systems Biology

■ Prof MAMITSUKA, Hiroshi

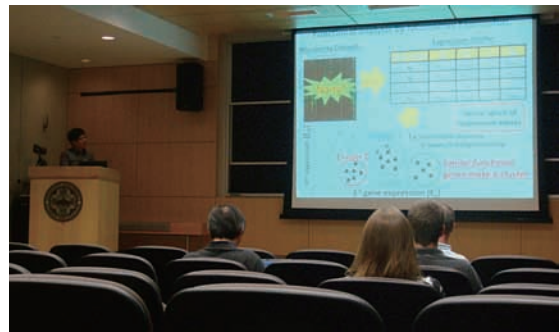
Bioinformatics Center launched JSPS International Training Program (ITP) named “International Research and Training Program on Bioinformatics and Systems Biology” at April 2009. This program supports international research/education activities of Bioinformatics Center, jointly conducted with Bioinformatics Program of Boston University and a systems biology research group in Berlin: 1) an annual workshop held in one of the three involved countries and 2) research stay of graduate students (and young researchers) in the counter-part research institutions.



A Bioinformatics Program's building (Life Science and Engineering Building, Boston University)



Participants to the 9th annual international workshop on Bioinformatics and Systems Biology (IBSB 2009)



A presentation at IBSB 2009

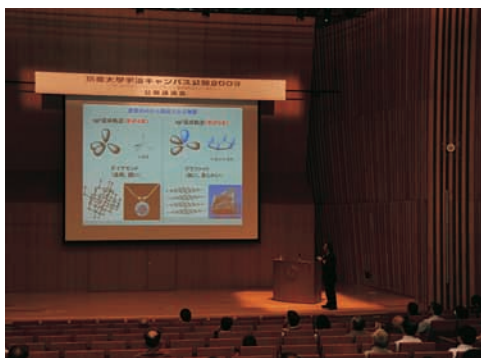
Opening of Uji Obaku Plaza



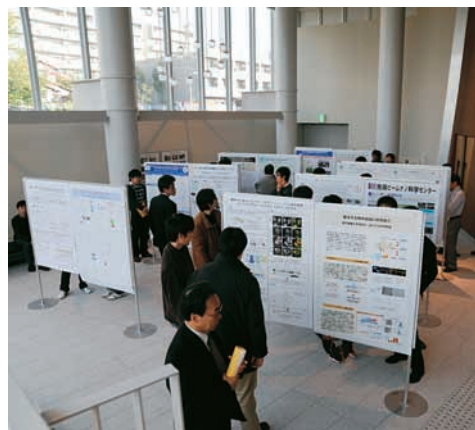
Uji Obaku Plaza

Uji Obaku Plaza opened on the 23rd of October 2009 in the Uji Campus of Kyoto University.

This new facility, with a lecture hall, restaurant, and meeting rooms, is expected to be used for research presentations and exchanges with the local community.



Public Lectures at KIHADA hall, Uji Obaku Plaza



Poster Presentation, the 109th ICR Annual Symposium at Foyer, Uji Obaku Plaza

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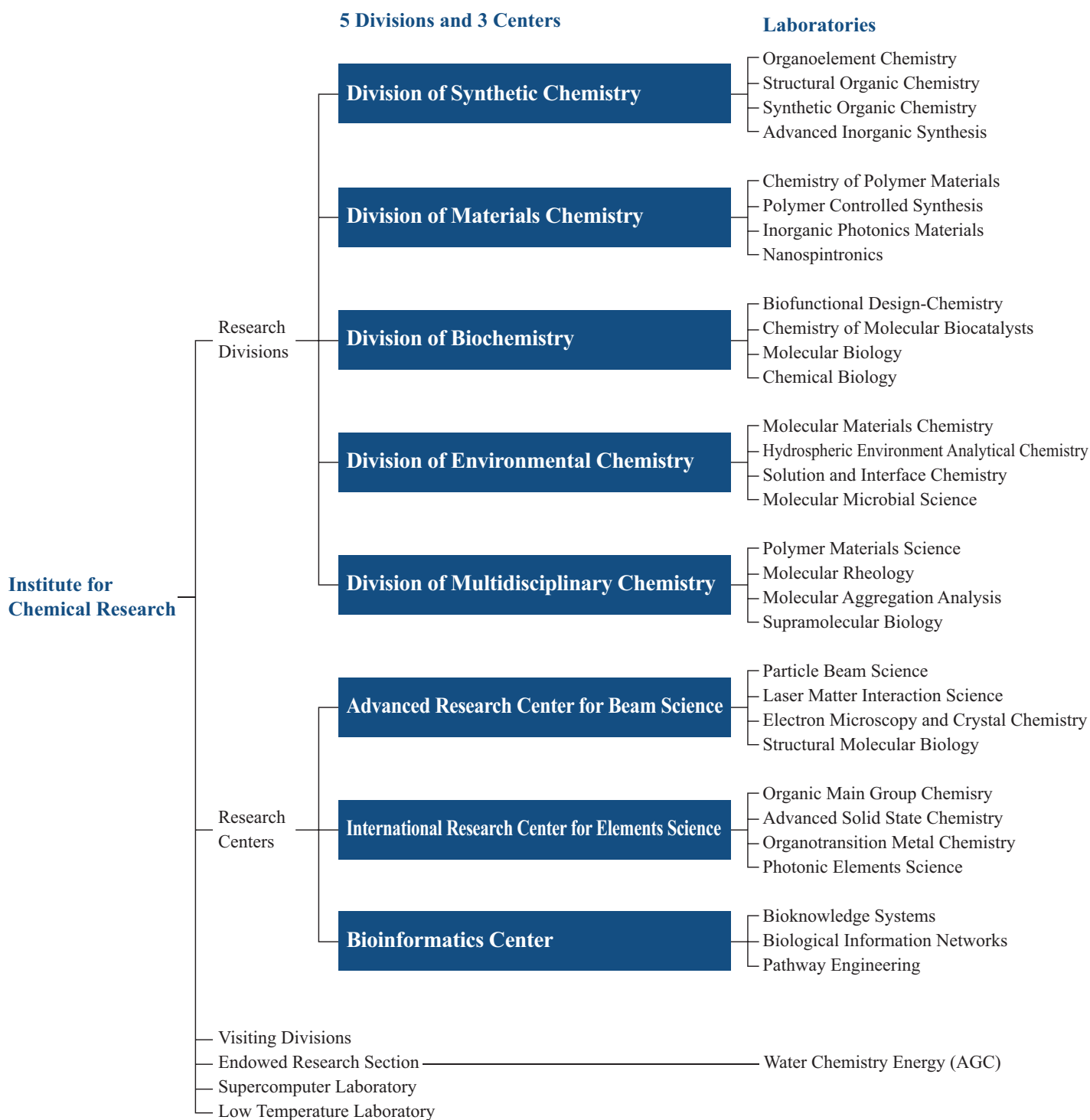
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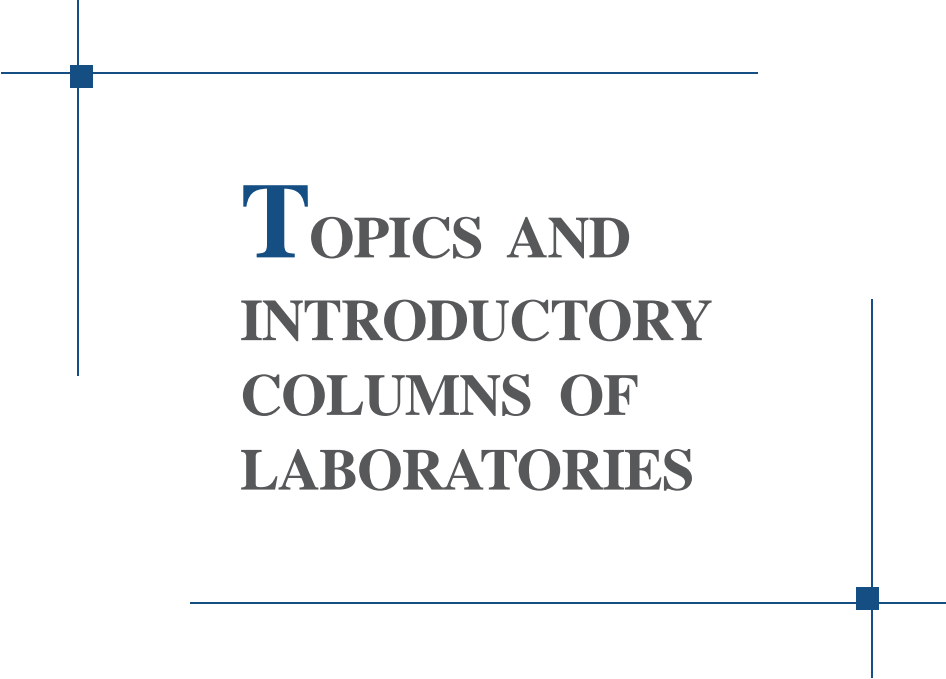
Abbreviations used in the columns

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



ORGANIZATION





TOPICS AND
INTRODUCTORY
COLUMNS OF
LABORATORIES

Division of Synthetic Chemistry - Organoelement Chemistry -

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



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SAKAI, Kiyomichi (M2)
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NODA, Naoya (M1)
SHIMIZU, Tomohiro (M1)

Visitors

Prof KOST, Daniel	Ben-Gurion University of the Negev, Israel, 15 October 2009
Prof ERKER, Gerhard	WestfälischeWilhelms-Universität, Germany, 18 September 2009
Prof GATES, Derek P.	University of British Columbia, Canada, 31 August 2009
Prof JONES, William D.	University of Rochester, USA, 25–26 August 2009
Prof ARNASON, Ingvar	University of Iceland, Iceland, 7 April–22 May 2009

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.

Research Activities (Year 2009)

Publications

Mizuhata Y, Sasamori T, Tokitoh N: Stable Heavier Carbene Analogues, *Chem. Rev.*, **109**, 3479-3511 (2009).
Yuasa A, Sasamori T, Hosoi Y, Furukawa Y, Tokitoh N:

Synthesis and Properties of Stable 1,2-Bis(metallocenyl)-disilenes: Novel $d-\pi$ Conjugated Systems with a Si=Si Double Bond, *Bull. Chem. Soc. Jpn.*, **82**, 793-805 (2009).
Tsurusaki A, Sasamori T, Tokitoh N: [4+2] Cycloaddi-

Stable 1,2-Bis(metallocenyl)disilenes: Novel d- π Conjugated Systems with a Si=Si Unit

1,2-Bis(metallocenyl)disilenes (metal: Fe or Ru) were synthesized for the first time and were characterized by spectroscopic and X-ray crystallographic analyses. On the basis of cyclic voltammograms, iron derivative was found to be a stable five-electron redox system with four steps, while ruthenium one showed four-step redox couples with four electrons. The UV/vis spectra and theoretical calculations for these disilenes suggested that they should be novel d- π conjugated systems containing a disilene unit.

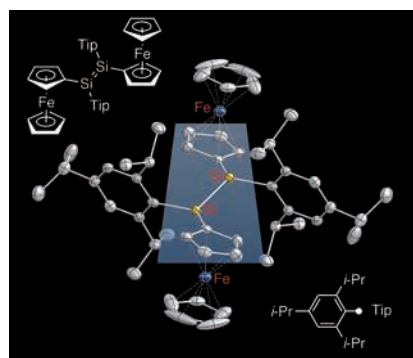


Figure 1. Structure of 1,2-Bis(ferrocenyl)disilene.

tion of 9-Anthryldiphosphene with Electron-Deficient Olefins: Transformation of a Diaryldiphosphene to Alkylaryldiphosphenes, *Organometallics*, **28**, 3604–3607 (2009).

Presentations

New Progress in the Chemistry of Silaaromatic Compounds, Tokitoh N, 14th Japan-Korea Joint Symposium on Organometallic and Coordination Chemistry, Nagoya, Japan, 9 October 2009 (invited).

Synthesis and Properties of Novel Functionalized Disilenes and a Stable Diaryldisilyne, Tokitoh N, 5th European Silicon Days, Vienna, Austria, 21 September 2009 (plenary).

Synthesis and Structures of Novel Rhodium Complexes Bearing a Schiff-base Type N,P-Chelating Ligands, Sasamori T, Matsumoto T, Tokitoh N, 12th International Symposium on Inorganic Ring Systems, Goa, India, 19 August 2009 (invited).

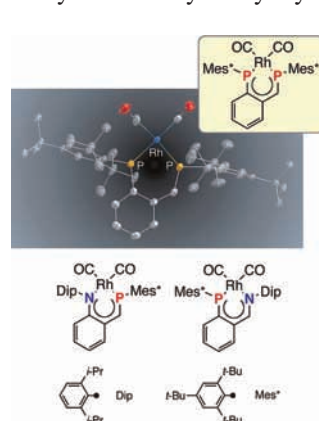
Some New Reactions of a Kinetically Stabilized Silabenzene and Isolation of a Stable 1,1'-Disila-4,4'-biphenyl, Tokitoh N, Tanabe Y, Mizuhata Y, 13th International Symposium on Novel Aromatic Compounds, Luxembourg, 22 July 2009 (invited).

Grants

Tokitoh N, Sasamori T, Mizuhata Y, The Chemistry of

Syntheses of Phosphorus Analogues of Schiff Base and Their Coordination Chemistry

Schiff-base type N,P- or P,P-chelating ligands, phosphorus analogues of imino-anilido ligands, were designed and synthesized as a new type of ligands toward transition metals, and the rhodium-carbonyl complexes bearing the novel imino-phosphido, phosphalkenyl-anilido, and phosphalkenyl-phosphido ligands were synthesized as stable crystalline compounds. Their structures were definitively revealed by X-ray crystallographic analysis, showing



the unique electronic features of the ligands. In addition, the effective trans-influence of the phosphorus atom was suggested on the basis of the structural parameters and spectroscopic features of the isolated complexes.

Figure 2. Rhodium Complexes Bearing Phosphorus Analogues of Schiff Base.

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 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.

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

Awards

Sasamori T, Progress Award in Silicon Chemistry, Japan, The Society of Silicon Chemistry, Japan, 31 October 2009.

Mieda E, The Best Poster Award, The 13th Symposium of the Society of Silicon Chemistry, Japan, 31 October 2009.

Yuasa A, Sasamori T, Tokitoh N, BCSJ Award, The Chemical Society of Japan, July 15, 2009.

Yuasa A, CSJ Student Presentation Award 2009, The 89th Annual Meeting of the Chemical Society of Japan, 13 April 2009.

Division of Synthetic Chemistry - Structural Organic Chemistry -

http://www.scl.kyoto-u.ac.jp/~kouzou/K_eHP_F/main.html



Prof
MURATA, Yasujiro
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YASUI, Hidefumi (M1)

KATSUYA, Satoshi (UG)

NOBORI, Masahiro (UG)

Visitor

Dr MARGETIC, Davor Rudjer Boskovic Institute, Croatia, 9 November 2009

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 by the use of transition metal complex.

Research Activities (Year 2009)

Publications

Horsewill AJ, Panesar KS, Rols S, Johnson MR, Murata Y, Komatsu K, Mamone S, Danquigny A, Cuda F, Maltsev S, Grossel MC, Carravetta M, Levitt MH: Quantum Translator-Rotator: Inelastic Neutron Scattering of Dihydrogen Molecules Trapped inside Anisotropic Fullerene Cages, *Phys. Rev. Lett.*, **102**, 013001 (4 pages) (2009).

Kohama Y, Rachi T, Jing J, Li Z, Tang J, Kumashiro R, Izumisawa S, Kawaji H, Atake T, Sawa H, Murata Y, Komatsu K, Tanigaki K: Rotational Sublevels of an Ortho-Hydrogen Molecule Encapsulated in an Isotropic C_{60} Cage, *Phys. Rev. Lett.*, **103**, 073001 (4 pages) (2009).

Presentations

Synthesis and Properties of Novel Open-Cage Fullerenes and Endohedral Fullerenes, Murata Y, Murata M, Kurotobi K, Kato K, Morinaka Y, Komatsu K, 13th International Symposium on Novel Aromatic Compounds, 20 July 2009, Luxembourg City, Luxembourg.

Synthesis and Reaction of Fullerene C_{70} Encapsulating Two Molecules of H_2 , Murata M, Maeda S, Morinaka Y, Murata Y, Komatsu K, 13th International Symposium on Novel Aromatic Compounds, 20 July 2009, Luxembourg

City, Luxembourg.

Synthesis and Properties of Novel Open-Cage C_{60} Derivatives, Kurotobi K, Murata M, Murata Y, The 11th International Kyoto Conference on New Aspects of Organic Chemistry, 12 November 2009, Kyoto, Japan.

Synthesis and Reaction of Fullerene C_{70} Encapsulating Two Molecules of H_2 , Murata M, Maeda S, Morinaka Y, Murata Y, Komatsu K, The 11th International Kyoto Conference on New Aspects of Organic Chemistry, 12 November 2009, Kyoto, Japan.

Grants

Murata Y, Synthesis of Novel Endohedral Fullerenes by Molecular Surgery Approach and Development of Their Function, PRESTO, Japan Science and Technology Agency, October 2005–March 2009.

Murata M, Synthesis and Properties of Carbon π -Systems with Curved Structures, Grant-in-Aid for Young Scientists (B), April 2007–March 2009.

Murata Y, Synthesis and Properties of Bowl-shaped π -Systems by Top-down Approach, Grant-in-Aid for Young Scientists (A), April 2008–March 2011.

Murata Y, Creation and Function of Spherical π -Space

Oxidation of the Open-Cage C₆₀ Derivative

Open-cage fullerene derivatives have drawn significant attention for the molecular surgical approach toward organic synthesis of endohedral fullerenes. Since the size of an opening is crucial for insertion of a small molecule inside the fullerene cage, chemical modification to make an opening larger and smaller is important. Previously, we reported chemical reaction on the rim of the opening for an open-cage C₆₀. However, we found that different reactions take place on its structural isomer **1** under the similar reaction conditions. Oxidation of **1** with one equiv of *m*-CPBA in CS₂ afforded open-cage C₆₀ **2** with a transannular bridge at the rim of the 13-membered ring opening. This compound is formed via oxidation of a sulfide group followed by addition of a water molecule to the carbonyl group on the five-membered ring on **1**. When a larger amount of *m*-CPBA (5 equiv) was used in *o*-dichlorobenzene instead of CS₂, another reaction took place to give open-cage C₆₀ **3** having a 14-membered ring opening with a lactone moiety. The size of opening was large enough for a neon atom to be inserted into the fullerene cage under high-pressure conditions.

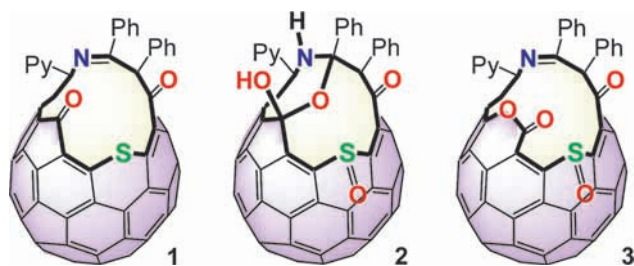


Figure 1. Structure of open-cage C₆₀ derivatives.

Expansion of 3D π -System with 2D π -System

It is very interesting to construct an extended π -system because unique photophysical and electrochemical properties are expected owing to the small HOMO-LUMO gap of the system. We recently synthesized open-cage C₆₀ derivative **1** by way of functionalization of the rim of an opening. UV-vis spectrum of **1** showed maximum absorptions at 330 (sh), 400 (sh), 450 (sh) and 730 nm extended to ca. 900 nm which is not seen for many examples of fullerene derivatives. When the redox properties were investigated by cyclic voltammetry in

benzonitrile, the first reduction wave was observed in less negative potential by 0.3 V from that of pristine C₆₀, indicating the lower-lying LUMO level. Furthermore, an irreversible oxidation wave was detected at 1.0 V, which was less positive than that of C₆₀. These properties are ascribed to expansion of 3D π -system of the C₆₀ moiety (colored in blue) with 2D π -system of the terphenyl moiety (colored in red) by sharing a part of π -system of the naphthalene moiety (highlighted in yellow).

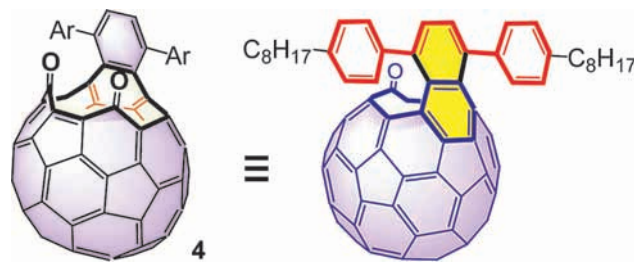


Figure 2. Open-cage C₆₀ derivative with expanded π -system.

Theoretical Investigation into Interaction of C₇₀ with Encapsulated H₂ Molecules

Is the reactivity of spherical π -system affected from inside? We have found that the equilibrium constant for Diels-Alder reaction of 9,10-dimethylantracene with (H₂)₂@C₇₀ is slightly smaller by 19% at 30 °C than that with H₂@C₇₀, studied by ¹H NMR analysis in *o*-dichlorobenzene-*d*₄. In order to get insights into the interaction of C₇₀ cage with encapsulated H₂ molecules, DFT calculations by MPWB1K/6-31G** were performed. When attention was paid to the optimized structures of C₇₀, H₂@C₇₀, and (H₂)₂@C₇₀, the difference in size was observed. The longer axis of (H₂)₂@C₇₀ is larger by 0.25%, whereas the shorter axis of (H₂)₂@C₇₀ is smaller by 0.30%, than that of H₂@C₇₀, respectively. Furthermore, small difference in the encapsulation energies of one and two H₂ molecules into C₇₀ as well as H₂C₇₀, as a model compound for the Diels-Alder adduct, were observed, which might account the experimental results.

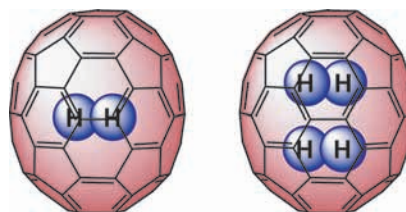


Figure 3. Endohedral C₇₀ encapsulating H₂ molecules.

Encapsulating an Active Small Molecule, Grant-in-Aid for Scientific Research on Innovative Areas “ π -Space”, December 2009-March 2014.

Award

Morinaka Y, The Best Poster Award, The 20th Symposium on Fundamental Organic Chemistry, 30 September 2009.

Division of Synthetic Chemistry - Synthetic Organic Chemistry -

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Scope of Research

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

Research Activities (Year 2009)

Publication

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

Presentations

Dynamic Molecular Recognition by an Organocatalyst: Glucose Specific Acylation, 11th International Kyoto Conference on New Aspects of Organic Chemistry, Kawabata T, 10 November 2009.

Practical Synthesis of Axially Chiral Amino Acid through Efficient Construction of Aza[5]helicenes, 22nd International Congress on Heterocyclic Chemistry (IHC-22), Furuta T, 3 August 2009.

Synthesis of Chiral Cyclic Ethers with Tetrasubstituted Carbon via C-O Axially Chiral Enolates, 7th Symposium on Organic Chemistry —The Next Generation—, Yoshimura T, 24 July 2009.

Catalytic Selective Acylation of Bifunctional Substrates, 96th Symposium on Organic Synthesis, Yoshida K, Kawabata T, 24 October 2009.

Binaphthyl Surrogates Possessing a Metal Center Directly Bound to the Chiral Axis, 34th Symposium on

Progress in Organic Reactions and Syntheses —Applications in the Life Sciences—, Hayashi K, Kawabata T, 17 November 2009.

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, 1 April 2007–31 March, 2009.

Kawabata T, Fine Organic Synthesis Based on Catalytic Regioselective Functionalization, Grant-in-Aid for Scientific Research (A), 1 April 2009–31 March 2012.

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.

Discrimination of Distal Enantiotopic Hydroxy Groups by Organocatalysis

Asymmetric desymmetrization of *meso*-1,2-diols, *meso*-1,3-diols, and prochiral 1,3-diols have been well established. However, the corresponding reactions of 1,5-diols and the longer analogues have rarely been developed because of their extreme difficulty. We have developed organocatalytic asymmetric lactonization of σ -symmetric 1,9-diols via discrimination of distal enantiotopic hydroxy groups with ~ 12 Å distance in between. Treatment of **2** with 10 mol% of **1** in the presence of *t*-Bu(*i*-Pr)NMe followed by benzoyl chloride gave **3** in 92% ee and 91% yield.

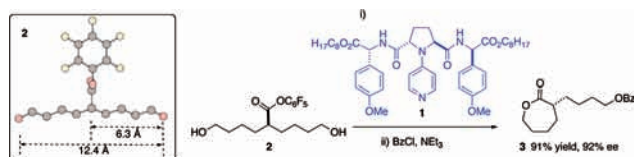


Figure 1.

Catalytic Kinetic Resolution of Axially Chiral Binaphthylamines

Nonenzymatic catalytic kinetic resolution of racemic amines has been extremely limited because uncatalyzed non-selective acylation competes significantly with catalyzed enantioselective acylation. We have developed the kinetic resolution of (\pm)-2,2'-disubstituted-1,1'-binaphthyl-8,8'-diamines with chiral C_2 -symmetric organocatalyst **4**. Treatment of the racemic aromatic amines with isobutyric anhydride in the presence of 10 mol% of **4** gave recovered unacylated amines in 86–98% ee at 61–71% conversion, which corresponds to the selectivity factor (*s*), 15–24. Based on the temperature-dependence of the enantioselectivity of the kinetic resolution, $\Delta\Delta H^\ddagger$ and $\Delta\Delta S^\ddagger$ between the acylation reactions for the fast-reacting (*S*)-isomer and the slow-reacting (*R*)-isomer were determined to be -2.9 kcal/mol and -7.8 kcal/mol, respectively. We assume that the acylation of the fast-reacting (*S*)-isomer proceeds via intermolecular hydrogen bonding between the catalyst and the NH_2 group of the (*S*)-isomer, where the reacting amino group is located close to the carbonyl group of the acyl-pyridinium intermediate. On the other

hand, the hydrogen bonding between the catalyst and the slow-reacting (*R*)-isomer does not make the reacting NH_2 group close to the carbonyl group, so that the (*R*)-isomer is expected to undergo direct acylation of the amino group without hydrogen-bonding interaction.

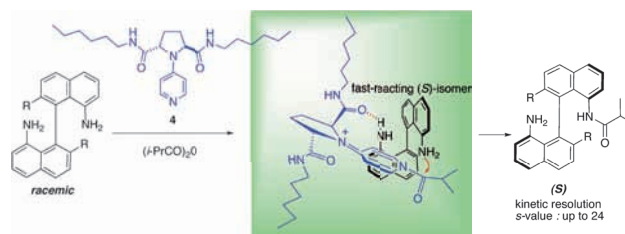


Figure 2.

Asymmetric Synthesis of Multisubstituted β -Lactams from α -Amino Acids

A method for asymmetric synthesis of multisubstituted β -lactams via intramolecular conjugate addition of the enolates derived from amino acid derivatives has been developed. Precursors **5** for β -lactam synthesis were readily prepared from α -amino acids via introduction of *p*-methoxyphenyl group into the nitrogen, acylation of the resulting amine with maleic anhydride, followed by esterification. Treatment of **5** ($\text{R}=\text{CH}_2\text{Ph}$) with cesium carbonate in ethanol at 0°C for 1 h gave a 1:1 mixture of *cis*- and *trans*-**6** in 95% and 96% ee, respectively, in a combined yield of 94%. Treatment of diastereomerically pure *trans*-**6a** ($\text{R}=\text{CH}_2\text{Ph}$, 96% ee) with cesium carbonate in ethanol at 20°C for 10 h gave a 12:1 mixture of *cis*- and *trans*-**6a** in 90% and 89% ee, respectively. Similarly, diastereomerically pure *cis*-**6a** ($\text{R}=\text{CH}_2\text{Ph}$, 92% ee) gave a 13:1 mixture of *cis*- and *trans*-**6a** in 84% and 77% ee, respectively, on treatment with cesium carbonate in ethanol at 20°C for 10 h. Thus, diastereoselectivity of the β -lactam formation was found to be thermodynamically controlled.

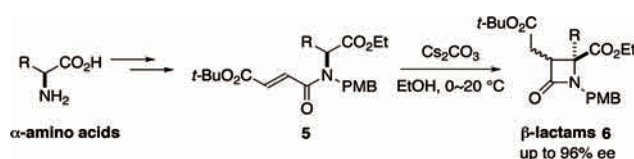


Figure 3.

Yoshimura T, Asymmetri Total Synthesis of Bioactive Natural Products via Planar Chiral Enolate, Grant-in-Aid for Young Scientists (B), 1 April 2009–31 March 2011.

Awards

Urano Y, Best Poster Award, “The Creation of a Peptide[2]catenane and D,L -Peptide Catalysts Based on Alternating D,L -Peptide Architecture”, The 29th Seminar on Synthetic Organic Chemistry for Young Scientists,

Kobe, 24 November 2009.

Urano Y, Impressive Oral Presentation Award, “Creation of a Peptide[2]catenane Based on Alternating D,L -Peptide Architecture”, The 39th Congress of Heterocyclic Chemistry, Kashiwa, 16 October 2009.

Urano Y, Impressive Poster Presentation Award, “Toward the Development of Unique Materials Based on Alternating D,L -Peptide Architecture”, The 5th Host Guest Chemistry Symposium, Utsunomiya, 30 May 2009.

Division of Materials Chemistry - Chemistry of Polymer Materials -

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Prof FUJIKAWA, Seizo Hokkaido University, 26 March 2009
Prof WATANABE, Junji Tokyo Institute of Technology, 27 March 2009

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 2009)

Publications

Tsujii Y, Nomura A, Okayasu K, Gao W, Ohno K, Fukuda T: AFM Studies on Microtribology of CPBs in Solvents, *J. Phys: Conf. Ser.* **184**, no. 012031 (2009).

Ladmiral V, Morinaga T, Ohno K, Fukuda T, Tsujii Y: Synthesis of Monodisperse Zinc-Sulfide Particles Grafted with CPB by Surface-Initiated Nitroxide-Mediated Polymerization, *Eur. Polym. J.*, **45**, 2788-2796 (2009).

Goto A, Nagasawa K, Tsujii Y, Fukuda T: Reversible Chain Transfer Catalyzed Polymerization (RTCP) with Alcohol Catalysts, *ACS Symp.*, **1023**, 159-168 (2009).

Presentations

Tsujii Y, New Development of CPBs as Novel Interfaces, NSYSU-KU Bilateral Symposium on Materials Chemistry, Kaohsiung, Taiwan, 22–23 September.

Ohno K, Applications of CPB/Particle Hybrids, PPC11,

Carins, Australia, 6–10 December.

Goto A, RTCPs with P, N, and O Catalysts. Materials of the Future, Melbourne, Australia, 15–17 February.

16 presentations, CPB meeting, Kyoto, 27 March.

6 Presentations, 58th Autumn Meeting, Soc. Polym. Sci., Jpn., Kumamoto, 16–18 September.

Grants

Tsujii Y, Fabrication of Novel Tribomaterials and Their Structural Analyses, Grant-in-Aid for Science Research (A), 1 April 2009–31 March 2012.

Tsujii Y, Development of High-Performance Battery System for Next-Generation Vehicles by NEDO, 1 July 2007–30 November 2009.

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,

Super-Lubrication Mechanism of Concentrated Polymer Brushes in Solvents

Previously, we revealed the super lubrication (ultra-low friction) between concentrated polymer brushes (CPBs) in good solvent. In order to clarify the lubrication mechanism in detail, the frictional coefficient μ was measured as a function of shearing speed v and solvent quality (controlled by mixing good and poor solvents), suggesting two mechanisms for swollen brushes; one is the boundary lubrication (with μ data little dependent on v), in which the non-interpenetrating interaction between the confronted brushes (specific to the CPB) plays an important role for ultra-low friction. The other is the hydrodynamic lubrication (with μ data dependent on v), in which the frictional property is related to the viscosity of solvent; interestingly, the data in this regime could be scaled by the degree of swelling. The better understanding of lubrication mechanism would open up a new strategy for the creation of novel tribomaterials.

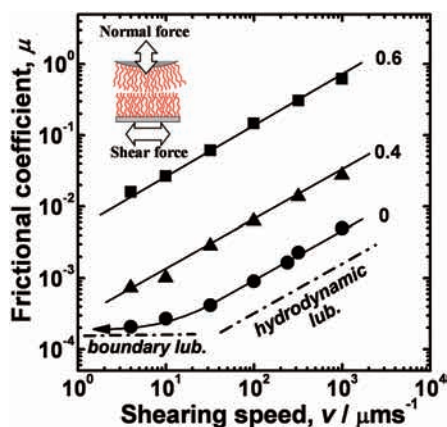


Figure 1. Plot of frictional coefficient μ vs shearing speed v for the CPB of poly(styrene) in isopropanol(IPA)/toluene(TOL) mixtures; the figures indicate the IPA content.

Carbon-Centered Compounds as a Novel Class of Catalysts for a Living Radical Polymerization

Carbon-centered compounds were successfully used as a novel class of catalysts for a living radical polymerization (RTCP). Low-polydispersity polystyrenes and functional polymethacrylates with predicted molecular weight were obtained with a fairly high conversion in a fairly short time. Notably, the catalysts include such common compounds as 1,4-cyclohexadiene (CHD) and diphenyl methane (DPM). Their commonness (hence low cost) and environmental safety may be attractive for practical applications. They also exhibited good tolerance to functional groups, being useful to a variety of functional monomers.

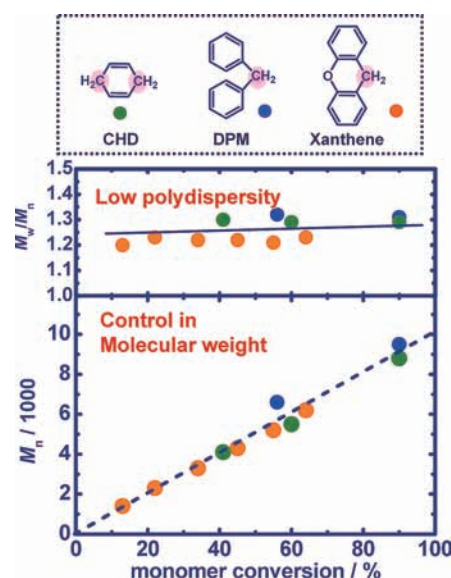


Figure 2. Plots of molecular weight (M_n) and molecular weight distribution (M_w/M_n) vs monomer conversion for the polymerizations of methyl methacrylate with carbon-centered catalysts.

1 September 2006–20 March 2010.

Tsujii Y, Development of Technology for Next-generation Fuel Cells by NEDO, 1 September 2008–20 March 2010.

Tsujii Y, Development of Novel Nanosystems by Hierarchically Assembling CPBs, CREST Program by JST, 1 October 2009–31 March 2015.

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

Goto A, Non-Transition-Metal Catalyzed and Photo-Induced LRP, 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, Development of New LRP, JST Promotion of Technology Research Partnership, 10 August 2008–31 July 2009.

Goto A, Fundamentals and Applications of New LRP, Kyoto Univ. Step Up Research Grant, 4 June 2009–31 March 2010.

Division of Materials Chemistry - Polymer Controlled Synthesis -

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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, and organometallic species 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 2009)

Publications

Yamago S, Ukai Y, Matsumoto A, Nakamura Y: Organotellurium-Mediated Controlled/Living Radical Polymerization Initiated by Direct C-Te Bond Photolysis, *J. Am. Chem. Soc.*, **131**, 2100-2101 (2009).

Kayahara E, Yamago S: Development of an Arylthio-bismuthine Cocatalyst in Organobismuthine-Mediated Living Radical Polymerization. Applications for Synthesis of Ultrahigh Molecular Weight Polystyrenes and Polyacrylates, *J. Am. Chem. Soc.*, **131**, 2508-2513 (2009).

Yamago S: Precision Polymer Synthesis by Degenerative Transfer Controlled/Living Radical Polymerization Using Organotellurium, Organostibine, and Organobismuthine Chain Transfer Agents, *Chem. Rev.*, **109**, 5051-5068 (2009).

Presentations

Organotellurium-Mediated Controlled/Living Radical Polymerization Initiated by Carbon-Tellurium Bond Photolysis, Yamago S, 2009 International Symposium on Nano Structures: Synthesis, Characterization and Application (3rd Korea-Japan Joint Seminar: Precisely Synthesis

and Applications), Gwanjyu, Korea, 7–10 October 2009 (invited lecture).

Recent Advances in Organoheteroatom-Mediated Controlled/Living Radical Polymerization, Yamago S, The 1st Federation of Asian Polymer Societies (FAPS) Polymer Congress, Nagoya, Japan, 20–23 October 2009 (invited lecture).

Taming Controlled/Living Radical Polymerization Reactions Using Organoheteroatom Compounds, Yamago S, 4th Pacific Symposium on Radical Chemistry, Shanghai, China, 19–22 November 2009 (invited lecture).

Organotellurium-Mediated Controlled/Living Radical Polymerization Initiated by Carbon-Tellurium Bond Photolysis, Yamago S, Ukai Y, Matsumoto A, Nakamura Y, 11th Pacific Polymer Conference, Cairns, Australia, 6–10 December 2009 (invited lecture).

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.

New Methods for Precision Polymer Synthesis by Controlled/Living Radical Polymerization (LRP)

LRP is now recognized as one of the most effective methods for the synthesis of advanced polymeric materials with well-defined structure. However, their application for the synthesis of high molecular weight polymers has been extremely difficult, because polymer end radicals are always subjected to irreversible termination reaction. We have developed a new cocatalyst, diphenyl (2,6-dimesitylphenylthio) bismuthine, in organobismuthine-mediated LRP. Both low and high molecular weight polystyrenes and poly(butyl acrylate)s with controlled molecular weights (M_n s) and low polydispersity indices (PDIs) were synthesized by the addition of a catalytic amount of the cocatalyst to an organobismuthine chain transfer agent (CTA). Structurally well-defined polymers with M_n s in the range of $1.0 \times 10^4 \sim 2.8 \times 10^6$ and PDIs of 1.06~1.43 were successfully prepared under mild thermal conditions.

We have also developed a photo-induced LRP in the presence of organotellurium CTAs by direct carbon-tellurium photolysis. The photo-activation of the organotellurium dormant species proceeded under weak intensity UV-vis light, and the polymerization proceeded at mild conditions, such as 0 °C. The polymerization shows high versatility in terms of monomer families and functional groups and, thus, provides a powerful method for the controlled synthesis of new polymer materials.

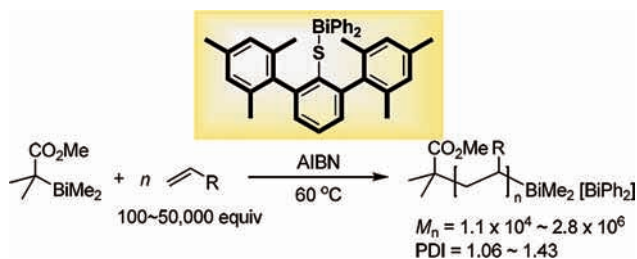


Figure 1. Controlled/living radical polymerization in the presence of a thio-bismuthine cocatalyst

Yamago S, Development of Photo-Induced Living Radical Polymerization Reaction and Its Applications, Torey Science Foundation, Torey Science and Technology Grant, 1 April 2008–31 March 2010.

Yamago S, Design and Synthesis of Novel Polymers for Drug Delivery, Uehara Memorial Foundation Research Grant, 1 April 2009–31 March 2010.

The First Synthesis of [8]Cycloparaphenylene

Cycloparaphenylenes have attracted the attention due to their unique structures having a distorted π system and potential applications in material science, since they are the simplest structural unit of armchair carbon nanotubes. Although they have a simple structure, their synthesis has been a significant challenge. We have succeeded in the synthesis of [8]cycloparaphenylene, which is the smallest cycloparaphenylene so far synthesized, based on a new synthetic route. Our synthetic strategy is to use a square-shaped tetra(*para*-substituted oligoaryl)platinum complex as a precursor for [4*n*]cycloparaphenylene. Once the complex is formed, multiple reductive elimination of platinum gives [4*n*]cycloparaphenylene. As a proof of principle for this strategy, we examined and succeeded in the synthesis of [8]cycloparaphenylene ($n = 2$). [8] Cycloparaphenylene possesses strong fluorescent emission at around 540 nm.

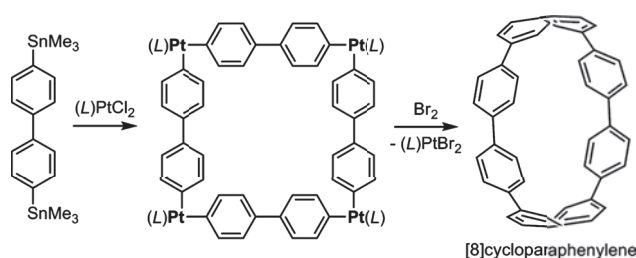


Figure 2. Synthesis of [8]cycloparaphenylene and its fluorescent emission in chloroform



Yamago S, Creation of Novel Nano-System through Hierarchization of High Density Polymer Brushes, CREST, 1 October 2009–31 March 2014.

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

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HATAYAMA, Yasuaki (UG)

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, photoluminescence 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-resolution NMR, thermal analysis, various laser spectroscopies and quantum chemical calculations.

Research Activities (Year 2009)

Publications

Kakiuchida H, Takahashi M, Tokuda Y, Yoko T: Rewritable Holographic Structures Formed in Organic-Inorganic Hybrid Materials by Photothermal Processing, *Adv. Funct. Mater.*, **19**, 2569-2576 (2009).

Tokuda Y, Tanaka Y, Takahashi M, Ihara R, Yoko T: Silicophosphate/silicophosphate Hybrid Materials Prepared by Solventless Ethanol Condensation, *J. Ceram. Soc. Japan*, **117**, 842-846 (2009).

Teixeira LAV, Tokuda Y, Yoko T, Morita K: Behavior and State of Boron in CaO-SiO₂ Slags during Refining of Solar Grade Silicon, *ISIJ INTERNATIONAL*, **49**, 777-782 (2009).

Presentations

Oka T, Tokuda Y, Takahashi M, Yoko T, "Quantitative Structure Analysis of Quadrupolar Nuclei in Amorphous Materials", Annual Meeting of the Ceramic Society of

Japan 2009, Japan, 16–18 March 2009.

Oku S, Tokuda Y, Takahashi M, Yoko T, Yamada T, Kitagawa H, "Solvent-free Synthesis and Application of Proton-conducting Organic-inorganic Hybrid Phosphosilicate Membranes", The 47th Symposium on Basic Science of Ceramics, Japan, 8–9 January 2009.

Grants

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

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

Tokuda Y, Iketani Science and Technology Foundation, April 2009–March 2010.

Tokuda Y, The Kyoto University Foundation, April 2009–March 2010.

Structure Engineering and Material Function Controlling of Organic-inorganic Hybrid Materials

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. Such materials are frequently prepared by using a sol-gel method because of their composition selectivity and low-temperature processibility. However, the sol-gel process is sometimes complicated, and it is difficult to obtain monolithic material because of crack formation during solvent evaporation.

Recently, an organic-inorganic silicophosphate hybrid has been obtained under a solventless, catalyst-free, low-temperature, one-pot condition by using orthophosphoric acid and organically modified chlorosilane. The following acid-base reaction (metathesis) took place: $\text{Si-Cl} + \text{P-OH} \rightarrow \text{Si-O-P} + \text{HCl}\uparrow$. The resultant viscous liquid was cooled down to an ambient temperature, producing a transparent monolithic hybrid material that contained an almost complete alternating polymer consisting of silicate and phosphate units and a high homogeneity in an intermolecular scale. The crack-free monolithic hybrid material was easily obtained because of the absence of solvent evaporation.

One can easily introduce organic dyes into the abovementioned hybrid material as it melts at temperatures less than 100 °C and possesses various organic groups. Additionally, rare earth ions and Au nanoparticles can be easily dispersed in this hybrid material because the

present material has copolymer structure consisting of silicate and phosphate units. This high solubility of both the organic and the inorganic functional centers is one of the advantages of the optical host material application. Another advantage of this organic-inorganic hybrid material is related to the low-temperature processibility of the material because the melting temperature of the material is less than 100 °C, the material can be used in a hot-emboss technique or photothermal fabrication in order to obtain photonic devices (Figure 1).

In this study, we developed another class of silicophosphate hybrid formation reaction that is based on solventless alcohol condensation without HCl production: $\text{Si-OEt} + \text{P-OH} \rightarrow \text{Si-O-P} + \text{EtOH}\uparrow$. The hybrid material shows low-melting property, as melting temperatures ranged from 50 to 110 °C where the organic dyes do not degrade. The functional centers such as the rare earth ions will disperse homogeneously in the alternating copolymer of silicate and phosphate as reported previously. Additionally, the chemical durability was much higher than that of the hybrids prepared by the acid-base reaction. Therefore, the present hybrid material is a good candidate of the optical host material for the organic and/or inorganic functional centers.

We also developed proton-conducting organic-inorganic hybrid phosphosilicate membranes using organically modified alkoxy silane and anhydrous vinylphosphonic acid (Figure 2). The membranes synthesized in the present study are crack-free, large-sized, and flexible, and they exhibit good thermal stability up to intermediate temperatures (~218 °C). The proton conductivities of the hybrids are as high as 5.2×10^{-3} S/cm at 85 °C under 80% RH.

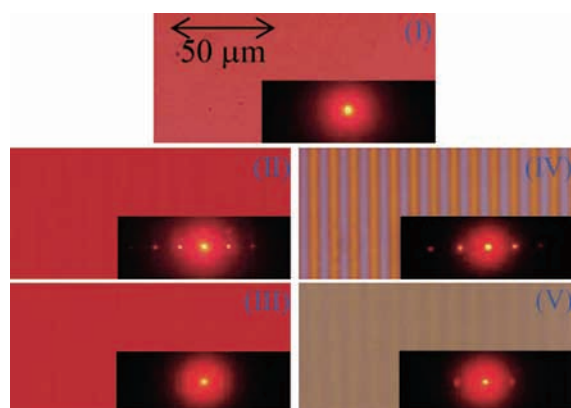


Figure 1. Snapshots of the optical grating images and diffraction patterns during the grating formation/decay process at lower (I, II–III) and higher (I, IV–V) irradiation intensities

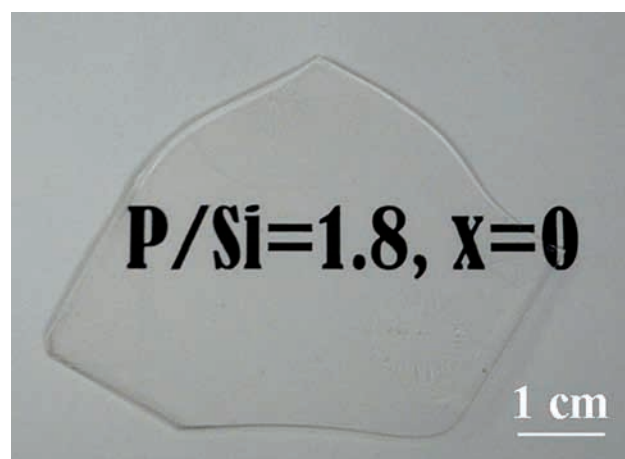


Figure 2. Photograph of an organic-inorganic hybrid phosphosilicate membrane. Crack-free and large-sized membranes were obtained.

Division of Materials Chemistry - Nanospintronics -

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Scope of Research

The conventional electronics utilizes only the “charge” of electrons, while the traditional magnetic devices use only “spin” degree of freedom of electrons. Aiming at the complete control of both charge and spin in single solid-state devices, a new field called *spintronics* is rapidly developing and impacting on information technology. By combining the atomic-layer deposition with nanofabrication, we focus on the development of spin properties of various materials and the control of quantum effects in mesoscopic systems for novel spintronics devices.

Research Activities (Year 2009)

Publications

Tanigawa H, Koyama T, Yamada G, Chiba D, Kasai S, Fukami S, Suzuki T, Ohshima N, Ishiwata N, Nakatani Y, Ono T: Domain Wall Motion Induced by Electric Current in a Perpendicularly Magnetized Co/Ni Nano-Wire, *Appl. Phys. Express*, **2**, 053002 (2009).

Delmo MP, Yamamoto S, Kasai S, Ono T, Kobayashi K: Large Positive Magnetoresistive Effect in Silicon Induced By The Space-Charge Effect, *Nature*, **457**, 1112 (2009).

Presentations

High DW Velocity in Co/Ni with Perpendicular Anisotropy, Ono T, IEEE International Magnetism Conference, 5 May 2009, Sacramento, USA.

Electric Field Manipulation of Magnetic Anisotropy in Ferromagnetic Semiconductors, Chiba D, IEEE International Magnetism Conference, 5 May 2009, Sacramento, California, USA.

Current-induced Domain Wall Motion in Perpendicularly

Magnetized Co/Ni Wires, Ono T, SPIE, NanoScience + Engineering, SpintronicsII, 2 August 2009, San Diego, USA.

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

Kobayashi K, Generation and Detection of Quantum Correlation in Semiconductor Nanostructures, Grand-in-Aid for Young Scientists (S), 1 October 2007–31 March 2012.

Chiba D, Study on the Electric-field Manipulation of Magnetization, Grand-in-Aid for Young Scientists (A), 1 April 2009–31 March 2012.

Current-induced Domain Wall Motion in Perpendicularly Magnetized Nano-wires

Motion of the magnetic domain wall (DW) induced by electric current in magnetic wires has been widely investigated because it is regarded as an important technique for future magnetic storage application as well as it provides exciting physics relevant to the interaction between spin current and local magnetic moment. A number of experiments and theoretical works have been reported so far. Among them, the systems with in-plane magnetization like NiFe are the most intensively investigated, although only a few works using perpendicularly magnetized systems has been reported.

Recently we have proven the domain wall motion induced by electric current in a Co/Ni nano-wire with perpendicular magnetic anisotropy. We detect the DW motion electrically by using the anomalous Hall effect. According to the theoretical calculations for the perpendicular magnetized systems, the decrease of the threshold current density for the DW motion has been predicted to be realized by the control of the wire dimension. As predicted, the threshold current density for the domain wall motion was found to decrease with decreasing the wire width. The observed behavior is consistent with the theory based on the spin transfer model and, therefore, our results are significant for future device application using DWs as well as understanding the physics of the current induced DW motion in perpendicularly magnetized materials.

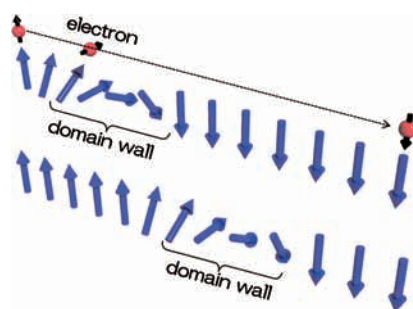


Figure 1. Schematic picture of the current-induced DW motion. The interaction between the conduction electrons and the DW plays the central role, which is called the spin-transfer torque.

New Feature of the Semiconductor Leader: Large Magnetoresistance in Silicon

Because silicon is one of the most intensively studied materials, on which the modern technology has been founded, one might think that no phenomenon remains to be discovered in it. Nevertheless, here, we report a new property of silicon; in a high electric field silicon shows large positive magnetoresistance between 0 T and 3 T more than 1,000 % at room temperature and 10,000 % at 25 K (see Figures in the bottom). The experiment on the lightly doped silicon reveals that when the carrier density decreases below $\sim 10^{13} \text{ cm}^{-3}$ the magnetoresistance exhibits linear dependence on the field between 3 T and 9 T in high electric fields. We propose that because of the quasi-neutrality breaking in the space charge effect, where no sufficient charge is present to compensate the electrons injected into the device, the electron motion becomes correlated with each other via the unscreened Coulomb interaction and thus the inhomogeneity is induced in silicon, yielding the unconventional non-saturating magnetoresistance as in the inhomogeneous semiconductors.

While large positive magnetoresistance at room temperature was achieved in the metal-semiconductor hybrid devices, it is now realized in a simpler structure in a way different from other known magnetoresistive effects. This novel effect can be utilized to develop new magnetic devices from silicon, which is expected to further advance the current silicon technology.

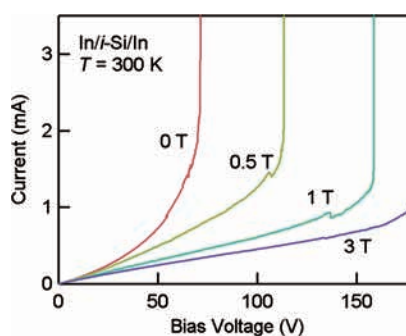


Figure 2. Large positive magnetoresistance in silicon induced by the space charge effect at room temperature.

Awards

Kobayashi K, the 3rd Young Scientist Award of the Physical Society of Japan, Experimental Study on the Controlling of the Coherence and the Many-body Effects of Electrons in Semiconducting Mesoscopic Systems, Physical Society of Japan, 28 March 2009.

Ono T, the 27th Osaka Science Prize, Pioneering Work on the Magnetization Control by Electric Currents, Osaka Prefecture, Osaka City and Osaka Science & Technology

Center, 11 September 2009.

Kasai S, Nakano K, Kondou K, Ohshima N, Kobayashi K, Ono T, MSJ Distinguished Paper Award, Time-resolved measurement of the Magnetic Vortex Core Dynamics by Using the TMR Effect, the Magnetic Society of Japan, 13 September 2009.

Chiba D, the 4th Condensed-Matter Science Prize, Experimental Study on the Electric Field Effect in Ferromagnetic Semiconductors, 29 November 2009.

Division of Biochemistry - Biofunctional Design-Chemistry -

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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 2009)

Publications

Inomata K, Ohno A, Tochio H, Isogai S, Tenno T, Nakase I, Takeuchi T, Futaki S, Ito Y, Hiroaki H, Shirakawa M: High-Resolution Multi-Dimensional NMR Spectroscopy of Proteins in Human Cells, *Nature*, **458**, 106-110 (2009).

Kobayashi S, Nakase I, Kawabata N, Yu H, Pujals S, Imanishi M, Giralt E, Futaki S: Cytosolic Targeting of Macromolecules Using a pH-dependent Fusogenic Peptide in Combination with Cationic Liposomes, *Bioconjug. Chem.*, **20**, 953-959 (2009)

Azuma Y, Imanishi M, Yoshimura T, Kawabata T, Futaki S: Cobalt(II)-Responsive DNA Binding of a GCN4-bZIP Protein Containing Cysteine Residues Functionalized with Iminodiacetic Acid, *Angew. Chem. Int. Ed.*, **48**, 6853-6856 (2009)

Presentations

“Chemical and Biological Factors that Affect the Internalization of Arginine-Rich Cell-Penetrating Peptides”, Futaki S, PepVec2009 Meeting on “Intracellular Delivery

of Therapeutic Molecules: From Bench to Bedside” Montpellier, France, 1 November 2009.

“Intracellular Delivery of Macromolecules Using Cell-Penetrating Peptides”, Nakase I, Kinki Bio-Industry Development Organization Follow-Up Seminar, Osaka, 11 November 2009.

“Creation of Zinc Finger-Based Artificial Transcription Factors”, Imanishi M, Department Seminar, School of Pharmacy, University of Maryland, Baltimore, USA, 21 November 2009.

“Physiological and Non-Physiological Factors Involved in the Internalization of Arginine-Rich Peptides”, Futaki S, 5th Peptide Engineering Meeting (PEM5), Barcelona, Spain, 27 October 2009.

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.

Imanishi M, Creation of Artificial Transcription Factors towards Construction of Artificial Genetic Circuit, Grant-

Cytosolic Targeting of Macromolecules Using a pH-Dependent Fusogenic Peptide in Combination with Cationic Liposomes

pH-Sensitive peptides and polymers have been employed as additives to enhance the cytosolic delivery of drugs and genes by facilitating their endosomal escape. However, little attention has been paid to the intracellular fate of these peptides and polymers. In this study, we explored the possibility of utilizing GALA, a pH-sensitive fusogenic peptide, as a cytosol-targeting vehicle. In combination with cationic liposomes, Lipofectamine 2000 (LF2000), the feasibility of this approach for the cytosolic targeting of proteins and nanoparticles was exemplified through the delivery of avidin (68 kDa) and streptavidin-coated quantum dots (15-20 nm) in serum-containing medium. The use of cationic liposomes is critical to enhance the cell-surface adhesion of the GALA conjugates and eventual endosomal uptake. Circular dichroism studies suggests that the GALA can be liberated from cationic liposomes at a reducing pH to form a helical structure and this may eventually lead to disruption of the endosomal membrane to achieve an efficient leakage of the GALA conjugates into the cytosol.

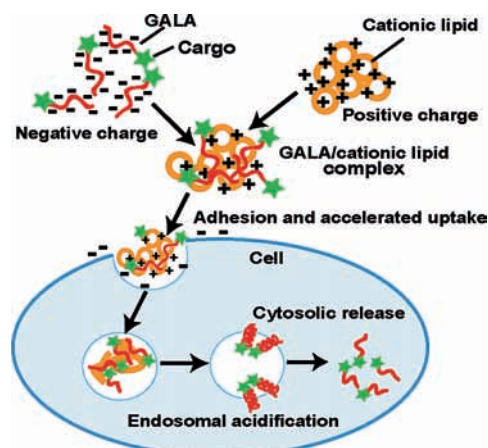


Figure 1. Concept of cytosolic targeting using GALA as an addressing vehicle in combination with cationic liposomes.

in-Aid for Young Scientists (B), 1 April 2008–31 March 2010.

Nakase I, Receptor Target and Efficient Internalization of Therapeutic Molecules into Cells Using Membrane Permeable Peptides, Grant-in-Aid for Young Scientists (B), 1 April 2009–31 March 2011.

Awards

Azuma Y, Best Poster Award, “Metal-Induced DNA-

Cobalt(II)-Responsive DNA Binding of a GCN4-bZIP Protein Containing Cysteine Residues Functionalized with Iminodiacetic Acid

Endowment of novel functions inducing that of metal switch can be attainable through structural design of peptides and proteins. We previously reported that helical peptides having a pair of iminodiacetic acid (Ida) derivatives of lysine at positions i and $i+2$ induce critical helix destabilization in the presence of metals to lead functional switch of peptides. However, due to the lack of the methodology to effectively introduce the Ida moieties at specific positions in proteins, the application of this concept has been limited to synthetic peptides.

We present a new method for introducing the Ida moieties into proteins. This employs specific modification of cysteines by treatment with a new functionalization agent, *N*-(2-tosylthioethyl) iminodiacetic acid (Ts-S-IDA). The practicability of this approach was exemplified through the metal-responding switching of the DNA binding of the yeast transcription factor GCN4-derived proteins bearing Ida moieties. Two pairs of Ida moieties were incorporated in the leucine zipper segment of the GCN4-bZIP protein in such a way that the Ida moieties of each pair were in i and $i+2$ positions. Complex formation of the Ida groups with Co(II) led to destabilization of the helical structure and thus enabled reversible switching of the binding of the protein to the target DNA.

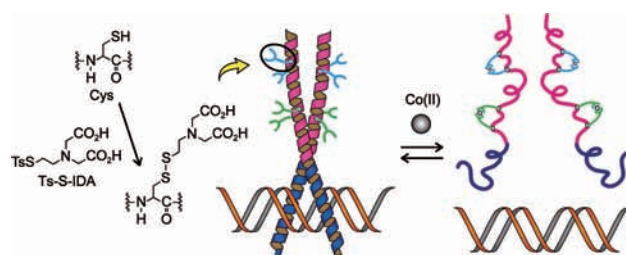


Figure 2. Preparation of Ida-modified cysteine in GCN4-bZIP protein mutant and conceptual scheme of metal-assisted DNA binding switch of GCN4-bZIP protein modified with Ida.

Binding Switch of bZIP Proteins Modified with Imino-diacetic Acid (Ida)” The 19th Symposium on Role of Metals in Biological Reactions, Biology and Medicine (SRM2009), Suita, 12 June 2009.

Nakamura A, Best Poster Award, “Creation of Artificial Zinc Finger-Type Transcription Factors towards Promoter Analysis of Clock Genes” The 16th Annual Meeting of Japanese Society for Chronobiology, Osaka, 27 October 2009.

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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) Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ -glutamylcysteine synthetase and γ -glutamyl transpeptidase, the key enzymes in glutathione biosynthesis and its metabolism, respectively. 2) Development of novel asparagine synthetase inhibitors and their application in cancer chemotherapy. 3) Development of intermediate analogue inhibitors of acyl-activating enzyme superfamily that plays pivotal roles in plant hormone homeostasis and secondary metabolite biosynthesis of plants.

Research Activities (Year 2009)

Publications

Ikeuchi H, Meyer ME, Ding Y, Hiratake J, Richards NGJ: A Critical Electrostatic Interaction Mediates Inhibitor Recognition by Human Asparagine Synthetase, *Bioorg. Med. Chem.*, **17**, 6641-6650 (2009).

Ogata M, Hidari KIPJ, Kozaki W, Murata T, Hiratake J, Park EY, Suzuki T, Usui T: Molecular Design of Spacer-N-Linked Sialoglycopolyptide as Polymeric Inhibitors against Influenza Virus Infection, *Biomacromolecules*, **10**, 1894-1903 (2009).

Presentations

Synthesis and Evaluation of Intermediate Analogue Inhibitors of 4-Coumaric Acid: CoA Ligase Involved in Secondary Metabolite Synthesis in Plants, Asai T, Naito Y, Yang Q, Hiratake J, 4th Annual Meeting of Japanese Society for Chemical Biology, Kobe, Japan, 18–19 May 2009.

Crystal Structure of Glutathione Biosynthetic Enzyme from *Streptococcus* sp. Complexed with Sulfoximine-Based Transition-State Analogue Inhibitor, Nakashima Y, Hibi T, Janowiak B, Griffith O, Hiratake J, Annual Meeting of Japan Society for Bioscience, Biotechnology, and

Agrochemistry 2009, Fukuoka, Japan, 27–29 March 2009.

Specific Affinity Chromatography Using Glycone Substrates as Ligand of Cellulases, Kameshima Y, Ogata M, Murata T, Totani K, Hiratake J, Usui T, Annual Meeting of Japan Society for Bioscience, Biotechnology, and Agrochemistry 2009, Fukuoka, Japan, 27–29 March 2009.

Development of Chemical Tools to Probe the Biosynthesis of Plant-Secondary Metabolites and Auxin Homeostasis -Design and Synthesis of Inhibitors of 4-Coumaroyl CoA Ligase (4CL) and CH3-, Hiratake J, The 2nd Nano-Bio Symposium 2009, Shizuoka, Japan, 6 March 2009 (invited).

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), 1 April 2007–31 March 2010.

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

Design and Synthesis of γ -Glutamyl Tranpeptidase Inhibitors

Glutathione (γ -Glu-Cys-Gly) plays a central role in detoxification of xenobiotics, and γ -glutamyl tranpeptidase (GGT) is a key enzyme in the metabolism of glutathione. We designed and synthesized transition-state analogue inhibitors highly mimicking glutathione to reveal the substrate-recognition mechanism of GGT. Structure-activity relationships disclosed that human GGT recognizes the stereochemistry of the Cys moiety and the phosphorous atom, and the negative charge at the Gly residue of the inhibitors. On the other hand, *E. coli* GGT showed low specificity particularly with respect to the recognition of the negative charge at the terminal Gly, and the result implied that the primary substrate of *E. coli* GGT is not glutathione. Mass spectrometric analysis showed that the inhibitor (R=Et) binds to the small subunit of GGT covalently in the manner that we anticipated. The crystal structure of a recombinant human GGT revealed that Lys562 strongly interacts with the negative charge at C-terminal Gly of glutathione and the inhibitors.

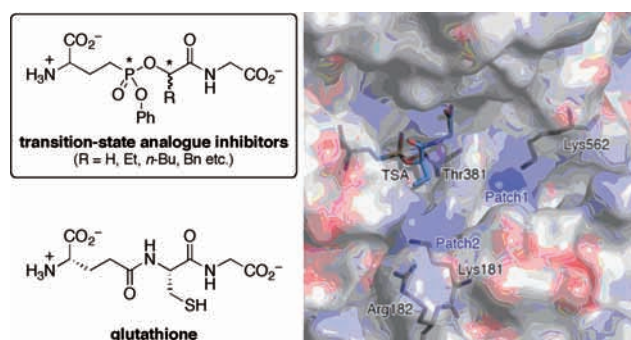


Figure 1. The structure of transition-state analogue inhibitors and substrate binding pocket of human GGT.

Inhibitors Targeting Asparagine Synthetase

Asparagine synthetase (ASNS) catalyzes the synthesis of Asn from Asp in an ATP-dependent manner. The inhibition of ASNS is highly important in enhancing and broadening the efficacy of asparaginase therapy of leukemia and cancer, and we have already developed the first potent *in vitro* ASNS inhibitor (**1**) that suppressed proliferation of asparaginase-resistant cancer cell line at 100-1000 μ M. In this study, we aim to increase *in vivo* activity of the original inhibitor by decreasing net negative charge, and synthesized sulfoximino-sulfamide and -sulfamate

based inhibitors (**2** and **3**) using rhodium catalyzed coupling of sulfoxide and sulfamide as a key step. Steady-state kinetic characterization of these compounds, however, has revealed the necessity of a localized negative charge on **1** that mimics that of the phosphate group in a key acyl-adenylate reaction intermediate.

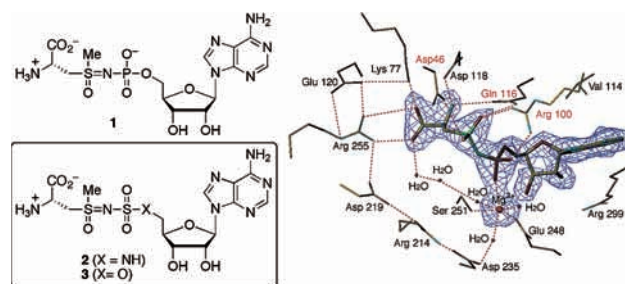


Figure 2. (Left) The structure of the original inhibitor (**1**) and newly synthesized inhibitors (**2** and **3**). (Right) X-Ray crystal structure of *E. coli* ASNS in complex with **1**.

Design of Specific Inhibitors of Acyl-activating Enzymes

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

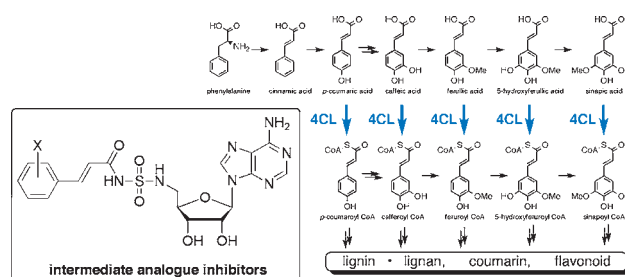


Figure 3. The outline of phenylpropanoid biosynthesis and the structure of intermediate analogue inhibitors.

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Dr LAMBREVA, Maya	National Research Council of Italy, Italy, 4–11 April 2009
Ms LOMBARDI, Benedetta	University of Rome La Sapienza, Italy, 9–14 June 2009
Prof QU, Li-Jia	College of Life Science, Peking University, China, 26–31 August 2009
Dr QIN, Genji	College of Life Science, Peking University, China, 26–31 August 2009
Dr HONG, Long	College of Life Science, Peking University, China, 26–31 August 2009
Dr LIU, Jingjing	College of Life Science, Peking University, China, 26–31 August 2009

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 2009)

Publications

Aoyama T: Phospholipid Signaling in Root Hair Development. *Root Hairs, Excellent Tools for the Study of Plant Molecular Cell Biology* (eds., Emons A.M.C., Ketelaar T, Springer, Berlin Heidelberg New York), 171-189 (2009).

Kusano H, Aoyama T: Mechanism Establishing and Sustaining the Polarity in Root Hair Morphogenesis: Focusing on Phospholipid Signaling. *Tanpakushitu Kakusan Koso*, **54**, 649-655 (2009).

Presentations

COP9 Signalosome: The Key Modulator of Signal Transduction in Plants and Mammals, Tsuge T, Invited Lecture at National Research Council of Italy, 9 February

2009 (Rome).

Phospholipid Signals for the Regulation of Plant Cell Polarity, Aoyama T, Symposium of Young Global Research Leader Promotion Program, 11 November 2009 (Shizuoka).

Grants

Aoyama T, Mechanism of Cytokinin Signal Transduction by the Response Regulator ARR1, Grant-in-Aid for Scientific Research (B) (2), 1 April 2009–31 March 2012.

Aoyama T, Role of Phospholipid Signals in Plant Cell Morphogenesis, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2009–31 March 2011.

Aoyama T, Signal Transduction from Nutrient Conditions

Involvement of Phospholipase D ζ 2 in Root Hydrotropism

Water deficiency is a frequently occurring difficulty for plants growing in natural fields. To survive this adversity, land plants are equipped with various means of altering their metabolism, morphology, and developmental processes. Of these, root hydrotropism, directional growth of roots toward moisture, is the most active means that plants can exert in the early stages of water deficiency. Root hydrotropism has been described for many plant species, including peas and maize. During the root hydrotropic response, the root cap senses a moisture gradient and transfers the signal to the root cell elongation zone, where asymmetric cell elongation results in root curvature. The involvement of calcium ions, auxin, and abscisic acid (ABA) in the signaling for this response has been revealed by genetic and physiological studies. From *Arabidopsis thaliana*, mutants specific to this response have been obtained. Moreover, in *Arabidopsis*, water deficiency is supposed to suppress root gravitropism to prioritize root hydrotropism. However, the mechanisms are still unclear,

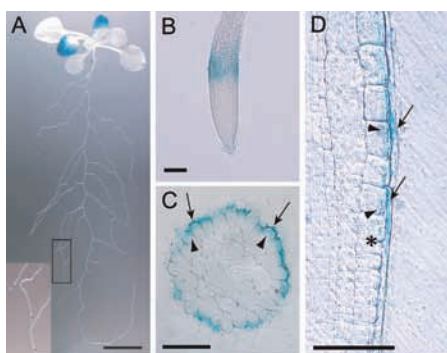


Figure 1. Histochemical analysis of the *PLD ζ 2* promoter. The *PLD ζ 2* promoter activity was histochemically analyzed using transgenic plants carrying the p*PLD ζ 2*-GUS gene at 10 days after germination. A: Seedling, B: Main root tip, C: Transverse section of a root in the transition zone, D: Longitudinal section of a root in the transition zone. An inset in (A) shows a magnified picture of the part encompassed by the square. Arrows and arrowheads indicate the lateral root cap and epidermal cells that exhibit GUS activity, respectively, in (C) and (D). An asterisk indicates the lower boundary of elongating epidermal cells in (D). Bar = 5 mm (A), 0.1 mm (B), and 0.05 mm (C, D).

not only for the establishment of root hydrotropism, but also the suppression of root gravitropism under water-deficient conditions.

We found that the promoter activity of the *Arabidopsis* phospholipase D ζ 2 gene (*PLD ζ 2*) was localized to epidermal cells in the distal root elongation zone and lateral root cap cells adjacent to them (Figure 1), and that exogenous ABA enhanced the activity and extended its area to the entire root cap. Although *pld ζ 2* mutant root caps did not exhibit a morphological phenotype in either the absence or presence of exogenous ABA, the inhibitory effect of ABA on gravitropism, which was significant in wild-type roots, was not observed in *pld ζ 2* mutant roots. In root hydrotropism experiments, *pld ζ 2* mutations significantly retarded or disturbed root hydrotropic responses (Figure 2). A drought condition similar to that used in a hydrotropism experiment enhanced the *PLD ζ 2* promoter activity in the root cap, as did exogenous ABA. These results suggest that *PLD ζ 2* responds to drought through ABA signaling in the root cap and accelerates root hydrotropism through the suppression of root gravitropism.

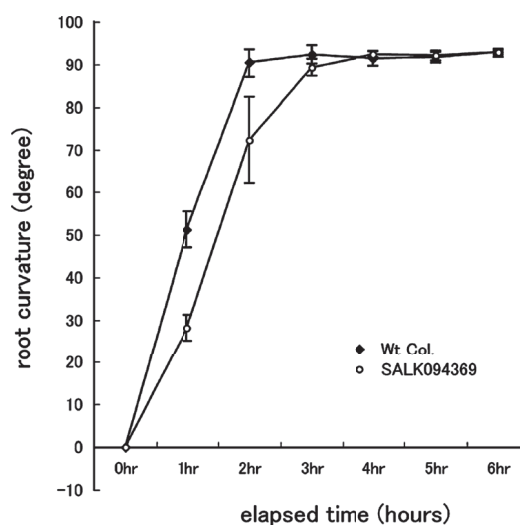


Figure 2. Hydrotropism analysis of *pld ζ 2* mutant roots. Wild-type (Wt Col.) and *pld ζ 2* mutant (SALK094369) plants were examined for their root hydrotropism under the moisture-gradient condition in a closed chamber. The angles of root curvature were measured every hour, and mean values were plotted. Error bars represent SE.

to Root Hair Morphogenesis, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2008–31 March 2010.

Tsuge T, Molecular Mechanism Conserved in Human Carcinogenesis Regulation and Plant Photomorphogenesis Regulation, Research Grant (Ito Kagaku Shinkou Foundation), 1 December 2008–31 March 2010.

Tsuge T, Understanding Plant Signal Transduction to Improve Solar Energy Usage, Research Grant (The Iwatani Naoji Foundation), 1 April 2009–31 March 2010.

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

Division of Biochemistry - Chemical Biology -

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Visitors

Vis Prof QUIOCHO, Florante A Baylor College of Medicine, U.S.A., 13 April–26 June 2009
Assoc Prof CHANG, Young-Tae National University of Singapore, Singapore, 5 October 2009

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 fundamental characteristics of human cells.

Research Activities (Year 2009)

Publications

Kamisuki S, Mao Q, Abu-Elheiga L, Gu Z, Kugimiya A, Kwon Y, Shinohara T, Kawazoe Y, Sato S, Asakura K, Choo H, Sakai J, Wakil SJ, Uesugi M: A Small Molecule that Blocks Fat Synthesis by Inhibiting the Activation of SREBP, *Chem. Biol.*, **16** (8), 882-892 (2009).

Yamazoe S, Shimogawa H, Sato S, Esko J. D, Uesugi M: A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth, *Chem. Biol.*, **16** (7), 773-782 (2009).

Jung D, Shimogawa H, Kwon Y, Mao Q, Sato S, Kamisuki S, Kigoshi H, Uesugi M: Wrenchanolol Derivative Optimized for Gene Activation in Cells, *J. Am. Chem. Soc.*, **131** (13), 4774-4782 (2009).

Presentations

Small Molecules that Boost Cell Adhesion and Growth, Uesugi M, The 3rd Asia-Pacific International Peptide Symposium (APIPS), Jeju, Korea, 9 November 2009.

Small Molecule Tools for Cell Biology and Cell Therapy, Uesugi M, (Invited) CBI-KSBSB JOINT CONFERENCE, Busan, Korea, 6 November 2009.

Small Molecule Tools for Cell Biology, Uesugi M, (Invited) Combinatorial Chemistry and Chemical Biology toward A New Paradigm for Drug Discovery (CCCB), Osaka, 25 September 2009.

Small Molecules that Control Gene Expression, Uesugi M, 7th AFMC International Medicinal Chemistry Congress

Small-molecule Tools for Cell Biology and Cell Therapy

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 fundamental characteristics of human cells. In human history, bioactive small molecules have been utilized in three major applications: as medicines, as agrochemicals, and as molecular tools for basic biological research. Our laboratory is interested in exploring another application of small molecules: tools for cell therapy. Through screening chemical libraries, we have been discovering unique synthetic molecules that modulate or detect fundamental characteristics of human cells. Some of such molecules may serve as tools for cell engineering or cell therapy as well as basic cell biological research.

Adhesamine

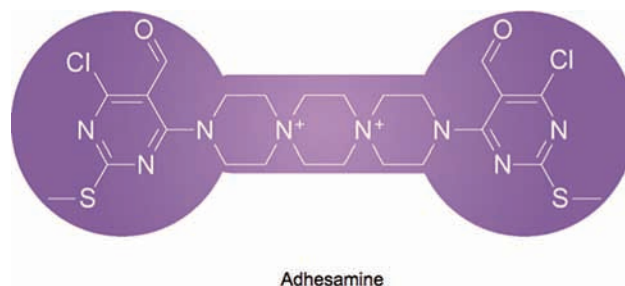
One such example is the small molecule that we named “adhesamine”. During an image-based phenotype screening of our chemical library, we noted a small molecule that boosts or enables the adhesion and growth of cultured human cells¹. This unique molecule, adhesamine, promotes cell adhesion and growth of a range of cell types,

including mouse iPS cells and primary cultured neurons. Chemical and cell biological experiments suggest that adhesamine targets selective cell-surface heparan sulfate for increasing cell adhesion and growth. Addition of adhesamine to the culture medium enables the adhesion of even floating lymphocytes to cell culture plates and the microinjection into them. Unlike poly-*L*-lysine, adhesamine induces apparently normal cell adhesion accompanied with organized actin structures and activation of focal adhesion kinase and ERK1/2 mitogen-activated protein kinases. In mouse hippocampal neurons, when compared with poly-*L*-lysine, adhesamine improves cell viability during long-term culture and enhances neuronal differentiation to matured neurons with less experimental periods².

Although the target of adhesamine is heparan sulfate (but not integrin), adhesamine often behaves like a small molecule version of fibronectin in cell culture and even in animals. Potential applications of adhesamine and its analogs will be discussed. Further synthetic and mechanistic studies of adhesamine may lead to the development of small molecule tools for cell biology and cell therapy.

(1) Yamazoe S, Shimogawa H, Sato S, Esko JD, Uesugi M: *Chem. Biol.*, 2009, **16**, 773-782 (2009).

(2) Hoshino M, Tsujimoto T, Yamazoe S, Uesugi M, Terada S: Submitted.



(AIMECS09), Cairns, Australia, 27 August 2009.

Synthetic Molecules that Control Gene Expression, Uesugi M, (Invited) 5th iCeMS International Symposium, Kyoto, 27 July 2009.

Grants

Uesugi M, Small-molecule Initiated Analysis of Cellular Signaling, Grant-in-Aid for Scientific Research (B), 1 April 2009–31 March 2012.

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.

Uesugi M, Practical Application of Small Molecules that Promotes Cell Adhesion, Adaptable and Seamless

Technology Transfer Program through Target-Driven R&D, 1 November 2009–31 October 2010.

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

Awards

Yamazoe S, Poster Prize, Discovery and Mechanism of Adhesamine, A Dumbbell-shaped Small Molecule that Promotes Cell Adhesion, 4th Annual Meeting of Japanese Society for Chemical Biology, 19 May 2009.

Yamazoe S, Poster Prize, A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth, The 25th Naito Conference, 11 September 2009.

Division of Environmental Chemistry - Molecular Materials Chemistry -

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Visitor

Dr OHIRA, Shino School of Chemistry and Biochemistry, Georgia Institute of Technology, USA, 27–29 October 2009

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 luminescence 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 2009)

Presentations

Solid-State NMR Analysis of Amorphous Materials and its Application for Organic Light-Emitting Diodes, Kaji H, The 7th International OLED and PLED Materials Workshop, 2009 Asian Symposium on Organic Materials for Electronics and Photonics (ASOMP 2009), Taipei, 15 December 2009 (Invited).

Solid-State NMR Analysis of Materials for Organic Light-Emitting Diodes and Organic Solar Cells, Kaji H, IMR Workshop on Organic Light-Emitting Devices, Sendai, 23 January 2009 (Invited).

Analysis of Carrier-Transports in Organic LEDs, Kaji H, ATP Symposium, Annual Meeting of the Chem. Soc. Jpn, Chiba, 28 March 2009 (Invited).

Synthesis of Phosphorus-Containing Materials and the Application to Electron-Transport Layers in Organic Light-Emitting Diodes, Fukushima T, Kaji H, 70th Annual Meeting, Jap. Soc. Appl. Phys., Toyama, 10 September 2009.

Simulation of Charge-Transports in TPD, a Hole-Transport Material, Kawaguchi H, Yamada T, Kaji H, 70th

Annual Meeting, Jap. Soc. Appl. Phys., Toyama, 10 September 2009.

Solid-State NMR Analysis of Structure and Dynamics of Polyfluorene, Shimahara Y, Fukushima T, Kiuchi Y, Kaji H, 9th Organic EL Symposium, Uji, 12 November 2009.

Analysis of Charge Transfer Integrals and Charge Transport Paths in CBP and TPD by Marcus Theory, Suzuki F, Yamada T, Sato T, Tanaka K, Kaji H, 9th Organic EL Symposium, Uji, 12 November 2009.

Formation of Liquid Crystals and the Magnetic Alignment of Tunicate Cellulose Nanofiber Suspensions, Hirai A, Nomura A, Tsujii Y, Tsuji M, Tosaka M, Kaji H, 58th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., Kumamoto, 17 September 2009.

Grants

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

Kaji H, Development of Solid-State NMR Methodology

Effects of Added Electrolytes on the Phase Separation Behavior in Aqueous Suspensions of Bacterial Cellulose Nanocrystals and on the Magnetic Alignment of the Chiral Nematic Phase

Effective utilization of cellulose as nano-materials is an important subject to create a sustainable society for the 21st century. Bacterial cellulose (BC) is produced by a gram-negative bacterium called *Gluconacetobacter xylinus* cultured in an aqueous medium containing carbon and nitrogen sources. The phase separation behavior in water suspensions has been studied for BC nanocrystals prepared by hydrolysis of BC with 60 wt% sulfuric acid at 51 °C for 1 h.¹ The suspensions separated into the upper isotropic and lower chiral nematic phases above 0.42 wt% of BC nanocrystals. The shape and size distributions of BC nanocrystals in both the phases were determined by transmission electron microscopy (TEM) and atomic force microscopy (AFM). The average size of the BC nanocrystals in the isotropic phase was 8.5 nm × 40 nm × 800 nm and the aspect ratio was 44. On the other hand, the average size of the BC nanocrystals in the chiral nematic phase was 9.8 nm × 54 nm × 1670 nm and the aspect ratio was 73. The surface charge densities were 0.051 and 0.055 e-nm⁻² for the isotropic and chiral nematic phases, respectively.

The effects of added NaCl (0–5.0 mM) on the phase separation behavior of the aqueous suspensions were investigated for a fixed total cellulose concentration of 3 wt% as shown in Figure 1.¹ The volume fraction of the chiral nematic phase had a minimum value at an NaCl concentration of ca. 1.0 mM. At NaCl concentrations ranging from 2.0 to 5.0 mM, the suspensions did not separate into two phases, but became entirely liquid crystalline, yet not chiral nematic. Figure 2 shows optical polarization micrographs of the anisotropic phase with the addition of NaCl. The size of the ordered domains in the anisotropic phase decreased with an increase in the NaCl concentration from 0 to 2.75 mM. At 2.75 mM, only tactoids were observed in the entire region. At 5.0 mM, chiral nematic domains were no longer observed. The chiral nematic pitch decreased with

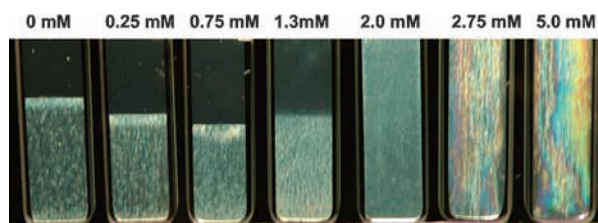


Figure 1. Effect of added NaCl on the phase separation behavior of the BC nanocrystals suspensions for a fixed total cellulose concentration of 3 wt% after 25 days of standing.

increasing concentration of added NaCl, reached a minimum value at approximately 0.75 mM, and then increased sharply with the NaCl concentration up to 2.0 mM.

The effects of added sodium chloride on the magnetic alignment of the chiral nematic phase of the suspensions are shown in Figure 3. Under a magnetic field of 9T at 20 °C for 24h, the helical axis of the chiral nematic phase of the suspensions without NaCl aligned parallel to the applied field. At 0.75 mM the helical axis of the chiral nematic phase aligned almost parallel to the applied field. However, the added NaCl more than 1.0 mM prevented the helical axis of the chiral nematic regions from aligning parallel to the field.

[1] Hirai A, Inui O, Horii F, Tsuji M: *Langmuir*, 25, 497-502 (2009).

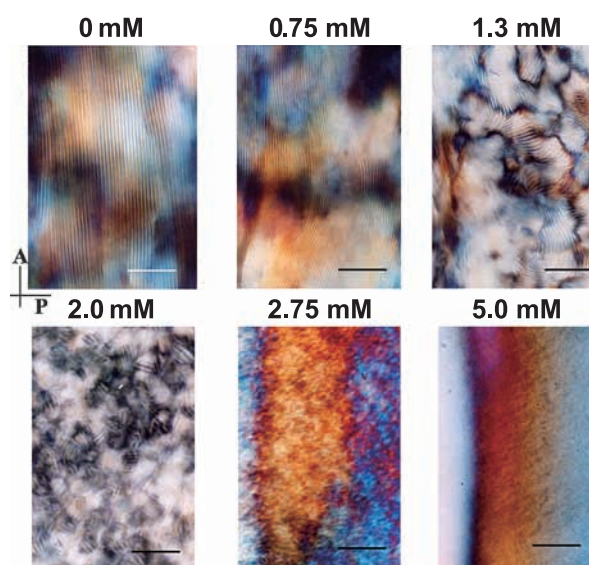


Figure 2. Optical polarization micrographs of the anisotropic phase with the addition of NaCl. The scale bars indicate 0.1 mm. Crossed polarizers are vertical and horizontal.

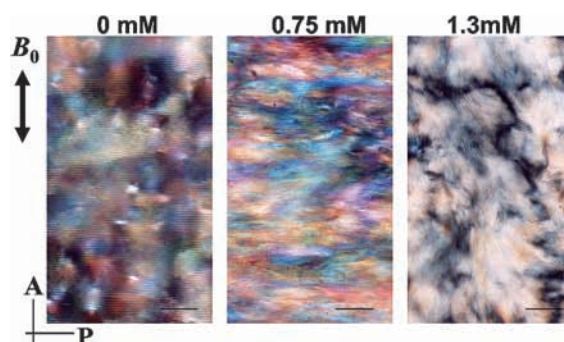


Figure 3. Effect of added NaCl on the magnetic alignment of the anisotropic phase of the suspensions with a total concentration of 3.0 wt%. A static magnetic field of 9T was applied to the samples at 20 °C for 24h. Scale bars indicate 0.1 mm.

for the Structure Analysis of Donor-Acceptor Supramolecules, Grant-in-Aid for Challenging Exploratory Research, 1 April 2009–31 March 2010.

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 -

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NAKASHIMA, Yusuke (M1)

WATANABE, Kazuya (M1)
VU, Thi Dieu Huong (RS)

Visitor

Dr BOWIE, A. R. Antarctic Climate & Ecosystems CRC, University of Tasmania, Australia, 30 March 2009

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 paleocene.

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

Research Activities (Year 2009)

Publications

Mukai H, Sohrin Y: 4,5-Bis(diphenylphosphinoyl)-1,2,3-triazole Ligand: Studies on Metal Complex Formations in Liquid-liquid Distribution Systems, *Inorganica Chimica Acta*, **362**, 4526-4533 (2009).

Hojo M, Ueda T, Hamada H, Chen Z, Umetani S: Conductometric Studies on Higher Ion-aggregation from Lithium Fluoroalkanoates in Propylene Carbonate and N,N-dimethylformamide, *J. Mol. Liquids*, **145**, 24-32 (2009).

Nakatsuka S, Okamura K, Takeda S, Nishioka J, Firdaus ML, Norisuye K, Sohrin Y: Behaviors of Dissolved and Particulate Co, Ni, Cu, Zn, Cd and Pb during a Mesoscale Fe-enrichment Experiment (SEEDS II) in the Western North Pacific, *Deep-Sea Res. II*, **56**, 2822-2838 (2009).

Presentations

Molecularly Imprinted Sol-gel Materials for the Separation of Metal Ions, Umetani S, Taguchi Y, Okabe T, Sohrin Y, 1st International Conference on Multifunctional, Hybrid

and Nanomaterials (Hybrid Materials 2009), 15 March 2009.

Tale of Oxygen in the Hydrosphere, Sohrin Y, Research Meeting of Geo Biotechnology Development Organization, 22 May 2009 (invited).

Do Phytoplanktons Dream of Iron?, Sohrin Y, Autumn Meeting of the Iron and Steel Institute of Japan, 9 September 2009 (invited).

Organic-inorganic Hybrid Adsorbents for Metal Ions Prepared by Ion Imprinting Synthesis, Umetani S, Meeting of the Union of Materials Engineering, Science Council of Japan, 19 October 2009 (keynote).

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.

Sohrin Y, Development of Precise Isotopic Analysis for Founding Heavy Stable Isotope-Marine Chemistry, Grant-in-Aid for Scientific Research (B), 1 April 1 2009–

Ocean Section of Dissolved Zr, Hf, Nb, Ta, Mo and W in the Southern and South Pacific Ocean

Ocean sections of trace elements and isotopes (TEIs) are important for understanding their geochemical cycles, anthropogenic contamination, and effect on ecology and global climate. Zr, Hf, Nb, Ta, Mo and W are adjacent metals in the periodic table. Their marine geochemistry is still poorly known¹. We are now studying the full-depth ocean sections of dissolved Zr, Hf, Nb, Ta, Mo and W along 170°W in the Southern and South Pacific Ocean. Seawater samples were collected during the KH-04-5 cruise of R/V Hakuho Maru (November 29, 2004 to March 22, 2005). By analyzing a large number of seawater samples (more than 250 samples from 12 stations²), we

are discovering the first meridional section of TEIs throughout ocean basins.

In general, Zr and Hf increase with depth (Figure 1). Nb and Ta show depletion in surface water (0–300 m depths) and enrichment in bottom water. The concentrations of Zr, Hf, Nb and Ta in surface water are higher at stations in the Southern Ocean than at the northern stations in the South Pacific Ocean. In deep water (2000–4000 m depths), Zr, Hf, Nb and Ta show gradual increase toward northern stations, coincident with the flow of seawater by global thermohaline circulation. Mo and W show uniform concentrations, regardless different water masses and ocean basins. Based on these findings, we are going to develop a new model of trace metal cycling in the ocean.

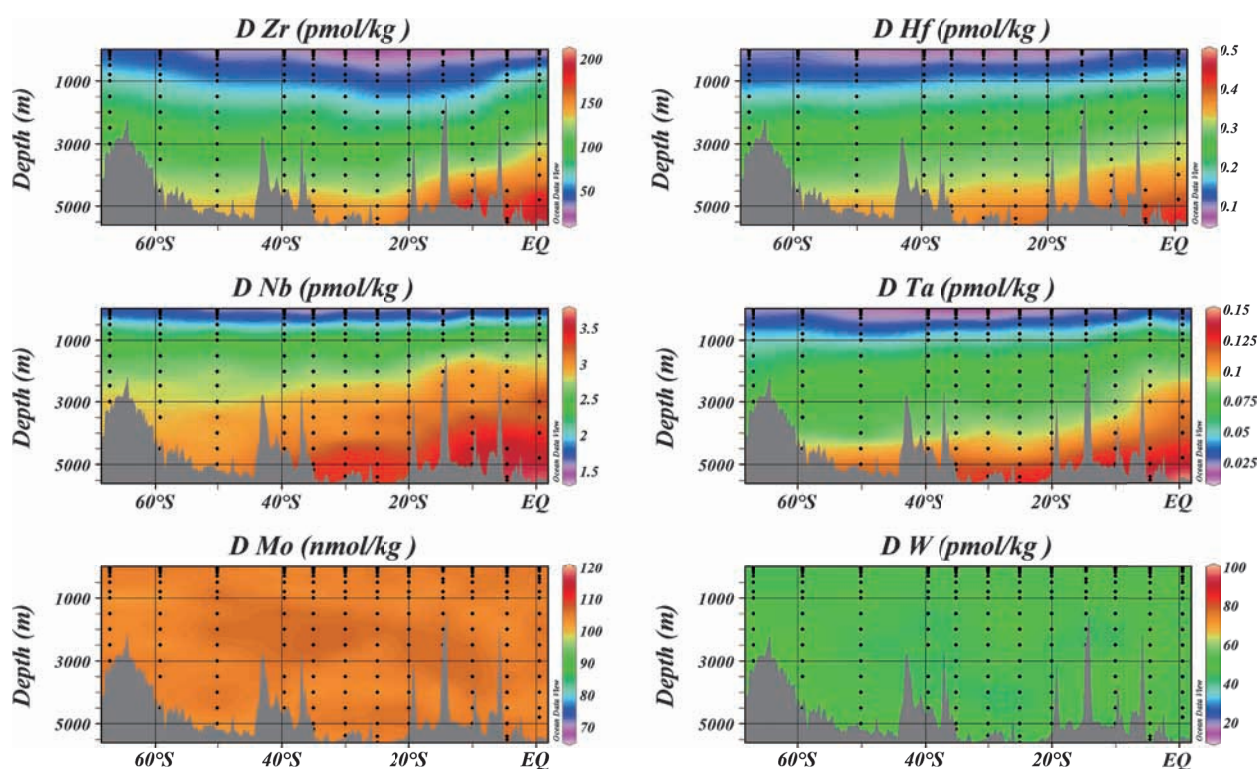


Figure 1. Full-depth ocean section of dissolved Zr, Hf, Nb, Ta, Mo and W in the Southern and South Pacific Ocean.

References:

1. M. Lutfi Firdaus *et al.*: *J. Oceanogr.*, **64**, 247-257 (2008).
2. M. Lutfi Firdaus *et al.*: *Anal. Chim. Acta*, **583**, 296-302 (2007).

31 March 2012.

Nakagawa Y, Stable Isotope Marine Geochemistry Using Molybdenum and Tungsten, Grant-in-Aid for JSPS Fellows, 1 April 2009–31 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.

Firdaus ML, Marine Geochemistry of High Field Strength Elements (Zirconium, Hafnium, Niobium, Tantalum, Molybdenum and Tungsten), Sasakawa Scientific Research Grant–The Japan Science Society, 1 April 2009–31 March 2010.

Division of Environmental Chemistry - Solution and Interface Chemistry -

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Visitors

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Prof ROSSKY, Peter J
Prof JUNGWIRTH, Pavel
Dr FEDOROV, Maxim

Pasteur Institute, France, 8–13 April 2009
University of Texas at Austin, 25–30 June 2009
Czech Academy of Science, Czech Republic, 8–14 July 2009
Max Planck Institute, Germany, 11 November 2009

Scope of Research

The structure, dynamics, and reaction of solutions with nano-scale inhomogeneity and/or with fine tunability are investigated by computer simulation, and statistical-mechanical theory of solutions, NMR spectroscopy, and vibrational spectroscopy. Solvation is systematically elucidated for ionic liquids and supercritical fluids from both the static and dynamic viewpoints, and noncatalytic 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 2009)

Publications

Yasaka Y, Wakai C, Matubayasi N, Nakahara M: Water as an In-situ NMR Indicator for Impurity Acids in Ionic Liquids, *Anal. Chem.* **81**, 400-407 (2009).

Yoshida K, Matubayasi N, Nakahara M: Self-diffusion Coefficients for Water and Organic Solvents in Extremely Low-density Supercritical States, *J. Mol. Liq.* **147**, 96-101 (2009).

Presentations

Free-Energy of Solvation in the Energetic Perspective, Matubayasi N, International Symposium on Multi-Scale Dynamics of Protein Complex Formation and Function, Tokyo, Japan, 14–16 July 2009.

Solvation Free Energy of Globular Proteins: A Molecular Dynamics Study, Saito H, Mizukami T, Matubayasi N, Nishikawa K, Nagao K, International Conference on

Computational Science 2009, Bali, Indonesia, 27–28 October 2009.

Grants

Matubayasi N, 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 ATP Hydrolysis, Grant-in-Aid for Scientific Research on Innovative Areas, 1 December 2008–31 March 2012.

Matubayasi N, MD and NMR Study of Molecular Binding into Lipid Membrane, Grant-in-Aid for Scientific Research (B), 1 April 2009–31 March 2013.

Free-Energy Analysis of the Configuration of Transmembrane Protein in Model Membrane

The configuration of a protein molecule in lipid-membrane environment plays important roles in the functions of bio-related membranes and the elaboration of drug-delivery systems. In the present work, we examine two contrast configurations of a transmembrane protein in a model membrane system. The purpose is to elucidate the factor to control the preferred configuration at atomic resolution. In the first configuration called the vertical configuration, the protein stays in the direction normal to the membrane surface, and in the second one called the horizontal configuration, it is buried in the membrane core, as shown in Figure 1. We investigate the effects of the different configurations in membrane by performing structural and free-energy analysis to reveal the roles of lipid and water.

The transmembrane protein employed in the present work is the transmembrane domain of glycoporphin-A. It consists of the residues 73-95 of glycoporphin-A, and holds the α -helical structure. The lipid molecule used is DMPC. The free-energy analysis was carried out using the method of energy representation.

The free-energy change of the protein binding into the membrane from vacuum is -133 kcal/mol for the vertical configuration and is -113 kcal/mol for the horizontal. The binding free energy is more favorable for the vertical configuration. The free-energy decomposition into the contributions from lipid and water shows that the lipid contribution is more favorable for the horizontal configuration. This is in agreement with the common notion of hydrophobicity. The water effect overturns the lipid one to stabilize the vertical configuration. Actually, the difference in the attractive interactions between the two configurations is by far larger for the protein-water interaction than for the protein-DMPC, and leads to the preference of the vertical configuration.

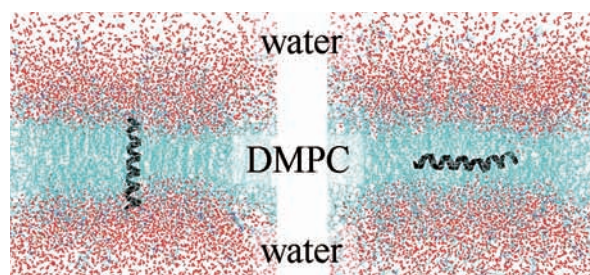


Figure 1. The vertical (left) and horizontal (right) configurations of the 23-residue protein in DMPC membrane system.

Slow Rotational Dynamics in Ionic Liquids

Ionic liquids are organic molten salts which are in the liquid state at ambient temperature. Ionic liquids are often in the deeply super-cooled liquid state at room temperature and show a glass transition at lower temperatures. They have very high viscosity compared with common organic solvents (~ 100 -fold even above the melting point) as a reflection of the strong Coulombic interactions between the positive and negative charges. The dynamics in ionic liquids is bimodal in the sense that the short-time local dynamics and the long-range slow dynamics are both significant.

The MD simulation was performed on the 248 ion pairs of [bmim⁺][Cl⁻] (the ionic liquid, 1-butyl-3-methylimidazolium chloride) with 8 water or benzene molecules. The initial configuration (NaCl-type lattice) was equilibrated in the *NPT* ensemble and then the trajectory was generated in the *NVT* ensemble. Several system temperatures were investigated in the range of 323-1250 K to analyze the temperature effect on the slow component of the rotational dynamics of the solutes.

The second-order rotational correlation function $C_2(t)$ of the C-H bond of benzene in [bmim⁺][Cl⁻] is shown in Figure 2 at several temperatures. The functional form of $C_2(t)$ at 323 K is far from exponential and is well fitted by the stretched exponential (linear function in the $\log t$ vs $\log(-\log C_2(t))$ plot) in the sub-ns time region. This is a glassy characteristic. The stretched exponential behavior is persistent above ~ 500 K (the decomposition temperature of ionic liquids in the real system). The crossover from the Gaussian-type relaxation in the short time region to the stretched-exponential type in the long time region is observed at ~ 1 ps.

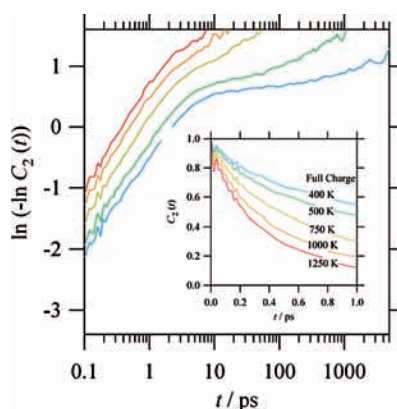


Figure 2. The second-order rotational correlation function of benzene in [bmim⁺][Cl⁻] on the logarithmic time scale. The temperatures are 1250, 1000, 750, 500, 400, and 323 K from top to bottom. The linear scale plot is shown in the inset.

Division of Environmental Chemistry - Molecular Microbial Science -

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MURAI, Ken (M2)

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TOYODA, Mayuko (M1)
WANG, Yu (M1)
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Visitors

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27 February 2008–17 February 2009

Dr ABE, Fumiyoishi Japan Agency for Marine-Earth Science and Technology, 20 October 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 2009)

Presentations

Cold-adaptation Mechanism of An Antarctic Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, Kurihara T, Xth SCAR International Biology Symposium, 27 July 2009.

Eicosapentaenoic Acid Plays An Important Role in Assembly of Cell Division Machinery of An Antarctic Sea Bacterium, *Shewanella livingstonensis* Ac10, Kawamoto J, Xth SCAR International Biology Symposium, 27 July 2009.

Phospholipids Involved in Cold Adaptation of An Antarctic Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, Kurihara T, NAIST Global COE International Symposium 2009 Environmental Adaptation, 13

November 2009.

Grants

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.

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.

Occurrence of a New Enzyme That Catalyzes the Degradation of Unsaturated Organohalogen Compounds

Enzymes catalyzing the conversion of organohalogen compounds are useful in chemical industry and environmental technology. A soil bacterium, *Pseudomonas* sp. YL, inducibly produced a protein named CAA67_YL when the cells were grown on 2-chloroacrylate (2-CAA). The *caa67_YL* gene encoded a protein of 547 amino acid residues, which showed weak sequence similarity to various flavoenzymes. We found that 2-CAA is converted into pyruvate when the reaction was carried out with purified CAA67_YL in the presence of FAD and a reducing agent under anaerobic condition, indicating that FADH₂ is required for the reaction. When the reaction was carried out in the presence of H₂¹⁸O, [¹⁸O]-pyruvate was produced. This result implies that CAA67_YL catalyzes the hydration of 2-CAA to form 2-chloro-2-hydroxypropionate, which is chemically unstable and probably spontaneously dechlorinated to form pyruvate. 2-Bromoacrylate, but not other 2-CAA analogs such as acrylate and methacrylate, served as the substrate of CAA67_YL. Thus, we named this new enzyme 2-haloacrylate hydratase. The enzyme is very unusual in that it requires the reduced form of FAD for hydration, which involves no net change in redox state of the coenzyme or substrate.

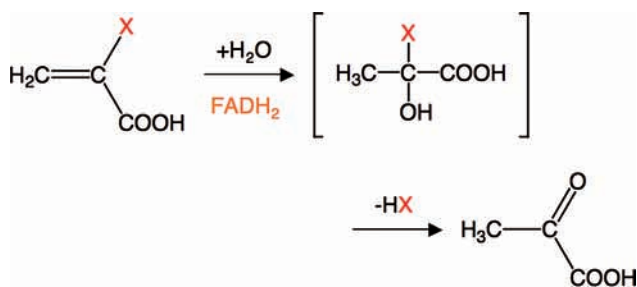


Figure 1. Reaction catalyzed by 2-haloacrylate hydratase.

Physiological Roles of Eicosapentaenoic Acid-containing Phospholipids in Cold Adaptation of an Antarctic Bacterium, *Shewanella livingstonensis* Ac10

Various bacteria favor cold environments including Polar Regions, glacier, and deep sea. Some cold-adapted bacteria produce polyunsaturated fatty acids (PUFAs), such as eicosapentaenoic acid (EPA) and docosahexaenoic acid, as a component of their membrane phospholipids, suggesting that PUFAs play important physiological roles in their cold adaptation. *Shewanella livingstonensis* Ac10, a cold-adapted Gram-negative bacterium isolated from Antarctic seawater, grows at range of temperatures from 4°C to 25°C and produces EPA at 4°C as a component of membrane phospholipids. The mutant lacking EPA showed significant growth retardation and became filamentous at 4°C but not at 18°C, indicating that the mutant has a defect in cell division at low temperatures. Interestingly, the EPA-less mutant developed multiple-intracellular membranes in its cell, suggesting that the deletion of EPA affects the physiological function of proteins involved in membrane biogenesis at low temperatures. FtsEX is supposed to be an ABC transporter composed of ATP binding domain (FtsE) and membrane-spanning domain (FtsX) and plays a role in the membrane-phospholipid transport at cell division site in Gram-negative bacteria. FtsE was localized to the cell membrane in the parent strain, but not in the EPA-less mutant. These results suggested that EPA supports the function and membrane localization of proteins related to cell division.

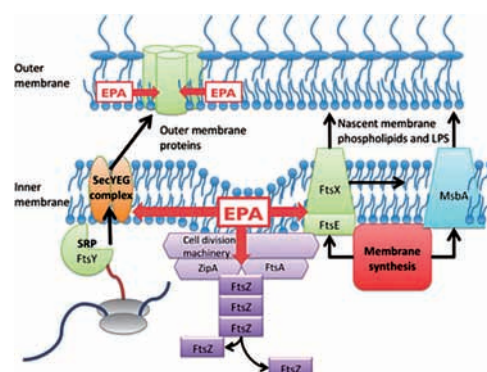


Figure 2. Schematic illustration of physiological roles of EPA in the cold adaptation of *Shewanella livingstonensis* Ac10.

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

Award

Kawamoto J, Poster Presentation Award, Physiological Role of Eicosapentaenoic Acid-containing Phospholipids in Refolding of a Cold-inducible Porin, Japan Society of Extremophiles, 28 October 2009.

Division of Multidisciplinary Chemistry - Polymer Materials Science -

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



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Visitors

Prof WU, Chi The Chinese University of Hong Kong, China, 1 May 2009
Prof GENZER, Jan North Carolina State University, USA, 1 June 2009
Prof RICHTER, Dieter Institut für Festkörperforschung, Forschungs Zentrum Jülich, Germany, 22 October 2009
Prof TANDON, Poonam University of Lackron, India, 18 December 2009

Scope of Research

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

Research Activities (Year 2009)

Publications

Hayashi Y, Matsuba G, Zhao Y, Nishida K, Kanaya T: Precursor of Shish-kebab in Isotactic Polystyrene under Shear Flow, *Polymer*, **50**, 2095-2103 (2009).

Ogawa H, Kanaya T, Nishida K, Matsuba G, Majewski P. J, Watkins E: Time-resolved Specular and Off-specular Neutron Reflectivity Measurements on Deuterated Polystyrene and Poly(vinylmethylether)blend Thin Films during Dewetting Process, *J. Chem. Phys.*, **131**, [104907-1]-[104907-7] (2009).

Presentations

Shear Induced Mesomorphic Phase Formation of Isotactic Polystyrene, Zhao Y, Matsuba G, Nishida K, Kanaya T, Annual Meeting, The Society of Fiber Science and Technology, Tokyo, 12 June 2009.

Distribution of Glass Transition Temperature in Polystyrene Multi-layered Thin Film, Kawashima K, Inoue R,

Matsuba G, Nishida K, Kanaya T, Annual Meeting, The Society of Fiber Science and Technology, Tokyo, 12 June 2009.

Gelation and Phase Separation of Methylcellulose Aqueous Solutions, Morita H, Tanaka K, Nishida K, Matsuba G, Kanaya T, The 55th Meeting of Polymer Science, Kobe, 17 July 2009.

Study of Crystallization and Mesomorphic Phase of Poly(Butylene-2,6-Naphthalate), Matsumoto N, Okada K, Nishida K, Kanaya T, The 55th Meeting of Polymer Science, Kobe, 17 July 2009.

Inelastic Neutron Scattering of Ultra-Thin Polymer Films, Kanaya T, Inoue R, Kawashima K, Matsuba G, Nishida K, IDMRSC 2009, Rome, 2 September 2009.

Fast Time-Resolved WAXD and SAXS Measurement of Mesomorphic Phase Formation of Isotactic Polypropylene, Nishida K, Okada K, Matsuba G, Ito K, Kanaya T, XIV International Conference on Small-Angle Scattering,

Critical Dissolution Ionic Strength of Chitosan Solution

Chitosan is derived from chitin, which is a major component of the shells of crustaceans, by the partial *N*-deacetylation, of its constituent glucosamine monomers. In our body, glucosamine is a principal constituent of the artrodial cartilage and as a consequence therefore chitosan is widely used as a health food supplement for the prevention and treatment of arthritic complaints. However, clarification of the fundamental properties of chitosan has been behind its applications. Here we have studied the formation and dissolution property of aggregates of chitosan in aqueous solution, with and without added salt using wide-dynamical range light transmittance measurements. A large hysteresis loop was found for both the formation of aggregates during cooling and the dissolution thereof during heating. In spite of the existence of the hysteresis, and regardless of the precise aggregation state and heating rate, the temperature at which the aggregates dissolved (namely the dissolution temperature) was uniquely determined for any given concentration of chitosan and NaCl. Further a critical dissolution ionic strength, below which no aggregation was detected, was established from the variation of dissolution temperature with ionic strength (Figure 1).

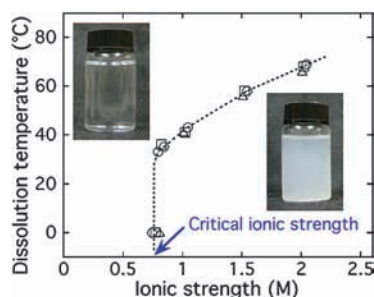


Figure 1. Dissolution temperature of aqueous chitosan as a function of ionic strength.

Oxford, UK, 17 September 2009.

Crystallization of Isotactic Polypropylene from Mesomorphic Phase during Heating with Constant Rates, Asakawa H, Nishida K, Okada K, Matsuba G, Kanaya T, Ogawa H, The 58th SPSJ Discussion (Autumn) Meeting, Kumamoto, 17 September 2009.

Crystallization Mechanism and Morphology of Polyamide-6, Kawabata J, Matsuba G, Nishida K, Kanaya T, The 58th SPSJ Discussion (Autumn) Meeting, Kumamoto, 17 September 2009.

Grants

Kanaya T, Higher Order Structure Formation in Induction Period of PLA Crystallization and External Fields,

Glass Transition of Polymer Thin Film

It is well known that physical properties of polymer thin films are quite different from those of bulk. One of the most fascinating topics is the thickness dependence of glass transition temperature (T_g) among them. The decrease of T_g with film thickness was reported for polystyrene thin films, however the detailed mechanism is still missing. Glass transition is believed to be dynamical transition, hence dynamical studies on polymer thin film give us some clues to the understanding of glass transition of polymer thin films. Therefore, we have studied the dynamics of polymer thin films by inelastic neutron scattering (INS) as a probe of dynamics. Figure 2 indicates the thickness dependence of T_g by INS with different energy resolutions and ellipsometry. We observed the decrease of T_g with thickness from ellipsometry, however the increase of T_g with the reduction of thickness was observed by INS although sample condition is same. In order to understand the contradiction, we used relaxation time map, which is based on the cooperatively rearranging region (CRR) concept, as shown in Figure 3. With this figure, we succeeded to explain contradiction reasonably.

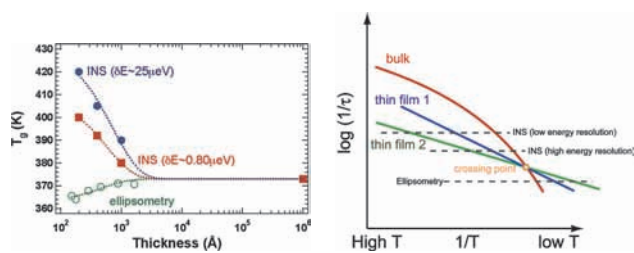


Figure 2. Thickness dependence of T_g evaluated from ellipsometry and inelastic neutron scattering (INS).

Figure 3. Schematic view of relaxation time map with the notion of CRR, which was used to explain our results.

Collaboration Research with Toyota Motor Corporation and Toyota CRDL., INC, 15 January 2003–30 September 2009.

Kanaya T, Polymer Crystallization and Control of Higher Order Structure Control through Non-equilibrium Intermediate States, Grant-in-Aid for Scientific Research (A), 1 April 2008–31 March 2011.

Award

Nishida K, The Award of the Society of Fiber Science and Technology, Japan, “In Situ Observation of Structure Formation in Fibers and Films”, The Society of Fiber Science and Technology, Japan, 10 June 2009.

Division of Multidisciplinary Chemistry - Molecular Rheology -

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



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KAWASAKI, Yoji (UG)

Visitors

Prof LODGE, Tim

Prof AHN, Kyung Hyun

Prof VAO-SOONGNERN, Visit

Prof SCHIEBER, Jay

Prof SUN, Kang

RAKKAPAO, Natthida

University of Minnesota, USA, 16 January 2009

Seoul National University, Korea, 25 January–22 February 2009

Suranaree University of Technology, Thailand, 13–14 March 2009

Illinois Institute of Technology, USA, 16–20 May 2009

Shanghai Jiao Tong University, China, 5–6 November 2009

Suranaree University of Technology, Thailand, 1 November 2008–31 October 2009

Scope of Research

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

Research Activities (Year 2009)

Publications

Watanabe H: Slow Dynamics in Homopolymer Liquids, *Polym. J.*, **41**(11), 929–950 (2009).

Masubuchi Y, Furuichi K, Horio K, Uneyama T, Watanabe H, Ianniruberto G, Greco F, Marrucci G: Primitive Chain Network Simulations for Entangled DNA Solutions, *J. Chem. Phys.*, **131**, [114906-1]-[114906-8] (2009).

Kawakita H, Uneyama T, Kojima M, Morishima K, Masubuchi Y, Watanabe H: Formation of Globules and Aggregates of DNA Chains in DNA/Polyethylene Glycol/monovalent Salt Aqueous Solutions, *J. Chem. Phys.*, **131**, [094901-1]-[094901-9] (2009).

Matsumiya Y, Inoue T, Iwashige T, Watanabe H: Dielectric Relaxation of Polymer/Carbon Dioxide Systems,

Macromolecules, **42**, 4712–4718 (2009).

Qiao X, Li W, Watanabe H, Sun K, Chen X: Rheological Behavior of Biocomposites of Silk Fibroin Fiber and Poly(ϵ -caprolactone): Effect of Fiber Network, *J. Polym. Sci. B: Polym. Phys.*, **47**, 1957–1970 (2009).

Okuda S, Inoue Y, Masubuchi Y, Uneyama T, Hojo M: Wall Boundary Model for Primitive Chain Network Simulations, *J. Chem. Phys.*, **130**, [214907-1]-[214907-7] (2009).

Sato H, Masubuchi Y, Watanabe H: DNA Diffusion in Aqueous Solution in Presence of Suspended Particles, *J. Polym. Sci. B Polym. Phys.*, **47**, 1103–1101 (2009).

Uneyama T, Masubuchi Y, Horio K, Matsumiya Y, Watanabe H, Pathak JA, Roland CM: A Theoretical Analysis of Rheodielectric Response of Type-A Polymer

DNA Diffusion in Aqueous Solution in Presence of Suspended Particles

Although nano-particles, which are comparable in size to polymer chains, are widely used as fillers to polymer matrixes for developing functional and high performance materials, the dynamics of polymers constrained between solid particles has not been well elucidated. In this study, dynamics of individual polymer under such condition was investigated with fluorescent microscopy using DNA solutions as model systems as shown in Figure 1.

For individual T4 and λ DNA molecules in aqueous suspensions of spherical polystyrene particles with diameter of 1 μm , it was found that i) the radius of gyration of DNA is independent of the particle volume fraction, ϕ_p ,

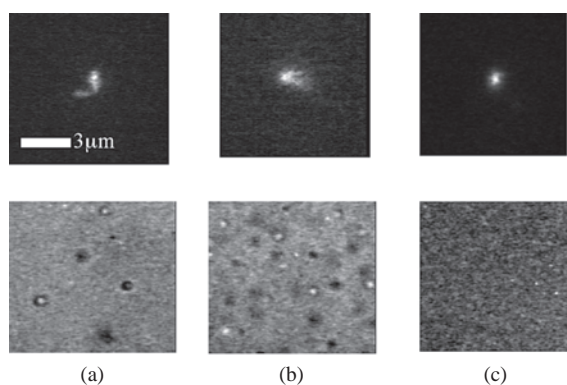


Figure 1. Typical snapshots of the probe T4-DNA (upper photos) and the particles (lower photos) at various particle volume fractions of (a) 4.9×10^{-4} , (b) 4.9×10^{-3} and (c) 9.8×10^{-2} .

Chains, *J. Polym. Sci. B Polym. Phys.*, **47**, 1039-1057 (2009).

Moriya M, Roschztardt F, Nakahara Y, Saito H, Masubuchi Y, Asakura T: Rheological Properties of Native Silk Fibroins from Domestic and Wild Silkworms, and Flow Analysis in Each Spinneret by a Finite Element Method, *Biomacromolecules*, **10**, 929-935 (2009).

Uneyama T: Coarse-Grained Brownian Dynamics Simulations for Symmetric Diblock Copolymer Melts Based on the Soft Dumbbell Model, *Nihon Reoroji Gakkaishi (J. Soc. Rheol. Japan)*, **37**, 81-90 (2009).

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, October 2006–March 2011.

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

ii) DNA diffusion is not sensitive to ϕ_p up to a certain critical ϕ_p where the average distance between particle surfaces is close to DNA size, and iii) the DNA diffusion becomes slower at higher ϕ_p . The diffusion coefficient of DNA was larger, by a factor of 2, in the suspensions at intermediate ϕ_p than in the corresponding confined geometry (channel/slit between fixed walls), while this difference asymptotically vanished with increasing ϕ_p (see Figure 2). This result suggested that the DNA diffusion in the suspensions with intermediate ϕ_p is accelerated by the particle motion. In fact, the diffusion coefficient measured for DNA in the suspensions was semi-quantitatively described by the Rouse constraint-release model considering the matrix effect on the probe chain diffusion.

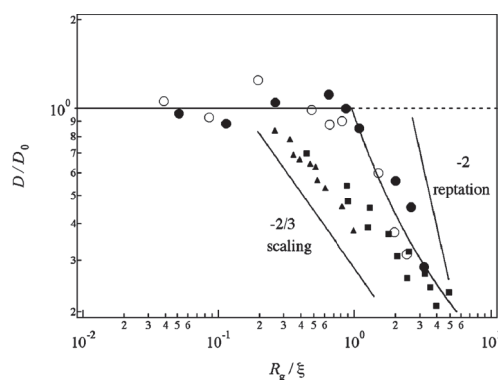


Figure 2. Normalized diffusion constant plotted against the normalized characteristic length of the constraint. Filled and unfilled circles are for T4 and λ DNA, respectively. Square and triangle are data for DNA in confined geometries. Solid lines are for the blob scaling theory and the reptation theory. Solid curves are prediction of the Rouse constraint-release model for T4 DNA. Horizontal broken line shows $D/D_0=1$.

March 2012.

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

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

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

Awards

Masubuchi Y, 2009 Award of Molecular Simulation Society of Japan.

Uno A, The Best Presentation Award in the 2009 Annual Meeting of the Society of Rheology, Japan.

Hiramoto K, The Best Presentation Award in the 2009 Autumn Meeting of the Society of Rheology, Japan.

Division of Multidisciplinary Chemistry - Molecular Aggregation Analysis -

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



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YOSHINAGA, Kengo (M1)

Visitor

DAOUD, Jamal McGill University, Canada, September–November 2009

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 spectroscopies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous structures in microcapsules, block copolymers, biological membranes and biological cells.

Research Activities (Year 2009)

Publications

Tsutsumi J, Sasamori T, Yoshida H, Tokitoh N, Sato N, Kato S, Muzikante I, Neilands O: A Noncentrosymmetric Crystal Structure of a Zwitterionic Compound, Pyridinium 5,7-Dihydro-5,7-dioxo-6H-cyclopenta[b]pyridin-6-ylide, Realized by Weak Hydrogen Bonds, *J. Mol. Struct.*, **920**, 52-60 (2009).

Asami K: Simulation of Dielectric Spectra of Erythrocytes with Various Shapes, *J. Phys. D: Appl. Phys.*, **42**, 135503 (2009).

Presentations

Murdey R, Sato N, The Growth Morphology of Ultrathin Films of Perylene-3,4,9,10-tetracarboxylic Dianhydride (PTCDA) on Rutile (110) Titanium Dioxide, Annual Meeting of Japan Society for Molecular Science 2009 (Nagoya, Japan), 23 September.

Sato N, Uchino Y, Yoshida H, Murdey R, Electronic Structure of Frontier States in an Evaporated Thin Film of Bis(catecholate)diboron, The 5th Workshop on Advanced

Spectroscopy of Organic Materials for Electronic Applications (Krusenberg, Sweden), 30 September.

Yoshida H, Sato N, Electronic Structure of Buried Interfaces at Organic/Metal Contacts Observed with Angle Resolved X-ray Photoemission Spectroscopy, The 5th Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (Krusenberg, Sweden), 1 October.

Grants

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.

Asami K, Monitoring of Cell Membrane Disruption and its Repair by Broadband Dielectric Spectroscopy, Grant-in-Aid for Scientific Research (C), 1 April 2009–31 March 2012.

Yoshida H, Preparation of Organic Thin Films with High Crystallinity Using the Supersonic Molecular Beam

A Noncentrosymmetric Crystal Structure of a Zwitterionic Compound, Pyridinium 5,7-Dihydro-5,7-dioxo-6*H*-cyclopenta[*b*]pyridin-6-ylide, Realized by Weak Hydrogen Bonds

An organic polar molecule with definitely deflected charge distribution within a single molecule is called a zwitterionic molecule and attracts much attention because of the potential applicability in optoelectronic devices. Pyridinium 1,3-dihydro-1,3-dioxo-2*H*-inden-2-ylide (PI) is a zwitterionic compound where the pyridine and indandione moieties are positively and negatively charged, respectively. Crystal structures of PI and its derivative compounds where a carbon atom at the 4th or 5th position of the indandione moiety of PI is substituted by a nitrogen atom, that is, 4N-PI or 5N-PI, respectively, were solved with X-ray diffraction analyses. Whereas PI and 5N-PI showed centrosymmetric crystal structures, 4N-PI demonstrated a noncentrosymmetric crystal structure where all the molecules orient to almost the same direction giving a polar crystal as shown in Figure 1. To elucidate the stability of such a polarized structure, we examined interatomic close contacts among the nearest neighbor molecules in

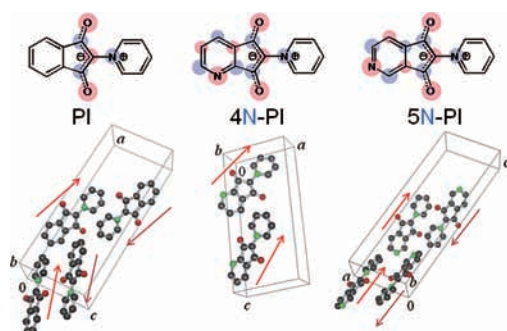


Figure 1. Molecular structures of PI, 4N-PI and 5N-PI and the respective molecular packing manners in the crystals. Blue and red circles indicate positively and negatively charged atoms, respectively. An arrow shows the direction of molecular dipole moment.

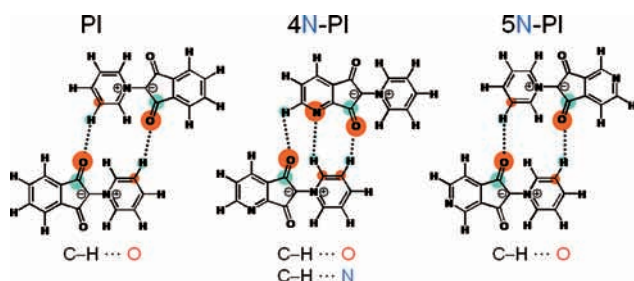


Figure 2. Molecular side-by-side interaction schemes of weak hydrogen bonds (shown by dotted lines) in PI, 4N-PI and 5N-PI crystals.

the crystals and calculated intermolecular interaction energies with relation to those contacts. As a result, the noncentrosymmetric crystal structure of 4N-PI turns out to be realized by a weak hydrogen bond in the C–H...N manner formed only in the case of this compound (Figure 2).

Effectiveness of ‘Thin-Layer’ and ‘Effective Medium’ Approximations in Numerical Simulation of Dielectric Spectra of Biological Cells

The dielectric spectrum of a biological cell suspension is calculated from electric potential distributions in a cell model, which are obtained by solving the Laplace equation. Since analytical solutions of the Laplace equation are limited to simple cell models such as spherical and ellipsoidal shell models, numerical simulation is needed for precise analysis of the dielectric spectrum. However, there are a few concerns when applying numerical techniques. Cells possess membranes of a thickness considerably smaller than the cell size, as well as a cytoplasm including membrane-bound intracellular organelles. The specific and complex cell morphology requires extra fine meshes, which results in considerable computational tasks, especially for 3D simulation. To solve the problems, the ‘thin-layer’ approximation (TLA) and the ‘effective medium’ approximation (EMA) were adopted. TLA deals with the membrane as an interface with zero thickness and the specific impedance of the membrane; it was applicable to cells and intracellular organelles of more than 0.1 μm in radius. EMA regards the composite cytoplasm (see Figure 3) as an effective homogeneous phase whose dielectric properties can be calculated separately. Numerical simulation of the dielectric spectra by the finite element method showed that TLA and EMA were both useful in greatly reducing computational tasks without losing accuracy.

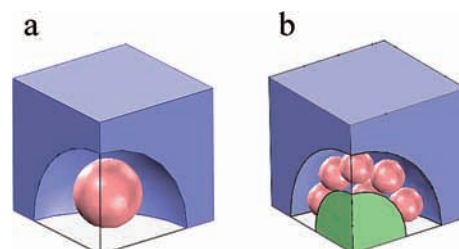


Figure 3. Composite cell models with (a) eight vesicles (red) and with (b) 48 small vesicles (red) surrounding one central large vesicle (green) in the spherical cytoplasm. The blue area is the external medium.

Deposition, The Murata Science Foundation, 1 July 2009–30 June 2010.

Yoshida H, Inverse-Photoemission Spectroscopy with

Zero Kinetic Energy Electrons for Measuring the Unoccupied Electronic States of Organic Semiconductors, JST PRESTO, 1 October 2009–31 March 2012.

Division of Multidisciplinary Chemistry - Supramolecular Biology -

<http://www.scl.kyoto-u.ac.jp/~umelab/index.htm>



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Assist Prof
KATO, Utako
(D Sc)



PD
JUNI, Naoto
(D Sc)

Res Associate (pt)

YAMAGUCHI, Yukiko

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KUBO, Akira (M2)

GOTO, Mina (M2)
YAMAMOTO, Masatoshi (M1)
TANABE, Aiko (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 2009)

Publications

Takeuchi K, Nakano Y, Kaneda M, Aizu M, Yamaguchi A, Kato U, Awano W, Kiyonaka S, Mori S, Yamamoto D, Umeda M: Changes in Temperature Preference and Energy Homeostasis in Dystroglycan Mutants, *Science*, **323**, 1740-1743 (2009).

Umeda M, Kato U: Physiological Function and Transport Machineries of Membrane Phospholipids, *J. Pharm. Sci.*, **09(suppl.1)**, 18 (2009).

Presentations

Umeda M, Cell Migration Control by Phospholipid Flippase, 4th International Conference on Phospholipase A2 and Lipid Mediators, 27 May 2009, Tokyo.

Ikenouchi J, Umeda M, Determination of Lipid Compositions of Particular Membrane Domains in Epithelial Cells, The 61st Annual Meeting of Japan Society for Cell Biology, 3 June 2009, Nagoya.

Kato U, Umeda M, Membrane Phospholipid Flip-flop and its Role in Cell Migration, The 82nd Annual Meeting of the Japanese Biochemical Society, 24 October 2009, Kobe.

Grants

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.

Ikenouchi J, Determination of Lipid Compositions of Particular Membrane Domains in Epithelial Cells, Grant-in-Aid for Young Scientists (A), 1 April 2009–31 March 2013.

Kato U, Basic Research for Development of Novel Anti-tumor Drugs Targeting Membrane Phospholipid Flip-flop, Grant-in-Aid for Young Scientists (B), 1 April 2009–31 March 2011.

Award

Ikenouchi J, Young Scientist Award for the Presentation, The 61st Annual Meeting of Japan Society for Cell Biolo-

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.

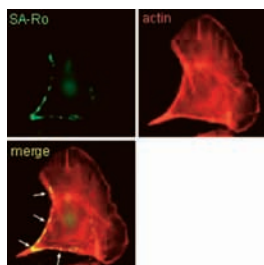


Figure 1. Cell-surface PE distributes in the inner leaflet of the ruffling membranes in migrating cells. The serum-stimulated cells were incubated with 10 $\mu\text{g/ml}$ PE-binding peptide (SA-Ro) for 30 min at 37 $^{\circ}\text{C}$, and then fixed and stained for SA-Ro and actin. Arrows indicate the 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).

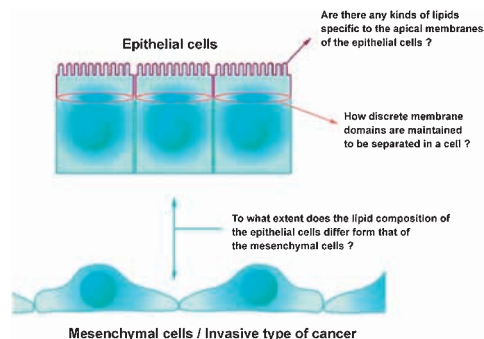


Figure 2.

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 $\Delta 9$ 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.

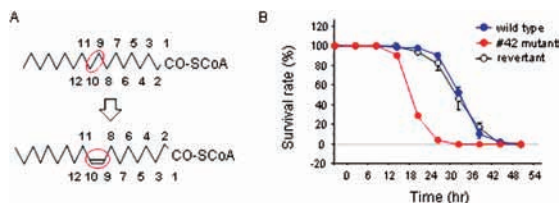


Figure 3. Starvation resistance was reduced in the *desat1#42* mutant flies.

A) Double bond introduction by stearoyl-CoA desaturase
B) Survival rate of wild type and *desat1#42* mutant flies during starvation

gy, Determination of Lipid Compositions of Particular Membrane Domains in Epithelial Cells, Japan Society for

Cell Biology, 3 June 2009, Nagoya.

Advanced Research Center for Beam Science - Particle Beam Science -

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Scope of Research

The Following Subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Ultra-low Emittance states of proton and Mg⁺ ion beams created by the electron cooling and laser cooling, respectively: Compression of the energy spread of laser-produced ion beams by an rf electric field for phase rotation: Research and development of permanent quadrupole magnets for final focusing of International Linear Collider (ILC) and for focusing of neutron beam: Development of electron-cyclotron resonance (ECR) ion source for small neutron source.

Research Activities (Year 2009)

Publications

Wakita A *et al.*: Characteristics of a Laser-produced Proton Beam Improved by a Synchronous RF Field, *Nucl. Instrum. Meth.*, **A599**, 15-19 (2009).

Suda T, Noda A *et al.*: First Demonstration of Electron-Scattering Using a Novel Target Developed for Short-Lived Nuclei, *Phys. Rev. Lett.*, **102**, 102501 (2009).

Noda A, Yogo A: Laser Ion Acceleration and Its Medical Application, *J. Vac. Soc. Jpn.*, **52**, 448-454 (2009).

Choi I.W., Iwashita Y, Noda A *et al.*: Ion Spectrometer Composed of Time-of-flight and Thomson Parabola Spectrometers for Simultaneous Characterization of Laser-driven Ions, *Rev. Sci. Instrum.*, **80**, 053302 (2009).

Ikegami M *et al.*: Radial Focusing and Energy Compression of a Laser-produced Proton Beam by a Synchronous RF Field, *Phys. Rev. ST Accel. Beams*, **12**, 063501 (2009).

Nishiuchi M, Souda H, Noda A *et al.*: Focusing and Spectral Enhancement of a Repetition-rated Laser-driven Divergent Multi-MeV Proton Beam Using Permanent Quadrupole Magnets, *Appl. Phys. Lett.*, **94**, 061107 (2009).

Presentations

Noda A *et al.*, Recent Approach to Crystalline Beam with Laser-Cooling at Ion Storage Ring, S-LSR, The 23rd Particle Accelerator Conference, 7 May 2009, Vancouver, Canada.

Iwashita Y *et al.*, Practical Applications of Permanent Magnet Multipoles, 21st International Conference on Magnet Technology, 20 October 2009, Hefei, China.

Souda H *et al.*, Experimental Approach for 2-dimensional Laser Cooling by Resonant Coupling at S-LSR, 64th Annual Meeting of Japanese Physical Society, 28 March 2009, Tokyo, Japan.

Grants

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

Transverse Laser Cooling of a Mg^+ Ion Beam Using Synchro-Betatron Resonance at S-LSR

Laser cooling of $^{24}Mg^+$ ion beams with the kinetic energy of 40 keV has been continued utilizing a transition between $3s^2S_{1/2}$ - $3p^2P_{3/2}$ at an ion storage and cooler ring, S-LSR. Up to now, longitudinal laser cooling of a coasting beam has been realized [1] and heat transfer from the horizontal degree of freedom to the longitudinal direction (direction of beam propagation) has been observed experimentally. Recent research activity on S-LSR has been concentrated to experimental verification of efficient reduction of transverse temperature by laser cooling with the use of "Synchro-Betatron Resonance".

Figure 1 shows the detection system of the transverse size of the $^{24}Mg^+$ ion beam with the use of a Cooled EB-CCD Camera (Hamamatsu Photonics C7190-11W), which detects the spontaneous emission from $^{24}Mg^+$ ion excited by a frequency-doubled dye-laser with a wavelength around 280 nm. The horizontal beam size has been observed changing the position of CCD in order to observe the coupling between the horizontal and longitudinal degrees of freedom in more straight forward way. The observed horizontal beam sizes depending on the CCD signal intensity are plotted in Figure 2. As the change of CCD signal intensity is mainly due to the ion beam intensity decrease due to beam life, it is found that reduction of the horizontal beam size is observed for synchrotron tunes between 0.068 and 0.077, estimated to be inside of the stopband of

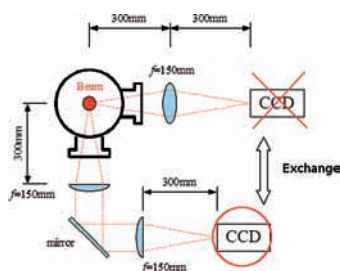
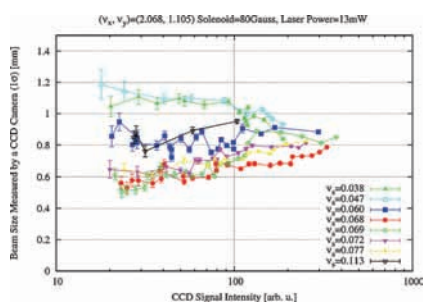


Figure 1. Observing system of the horizontal size of $^{24}Mg^+$ ion beam detecting spontaneous emissions from the ion excited by a laser with the use of a Cooled EB-CCD Camera.

Figure 2. Dependence of the horizontal beam size on the CCD signal intensity, which is considered to reduce according to passage of time due to the life time of the ion beam. Horizontal beam size reduction is observed selectively for synchrotron tunes between 0.068 and 0.077.



and Neutron Optics, Grant-in-Aid for Scientific Research, (A) (1), 1 April 2006–31 March 2010.

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.

Synchro-Betatron coupling resonance although its center is a little bit shifted to a higher tune side, which is a scope for further investigation.

Qualification of Laser-produced Ion Beam both in Radial and Longitudinal Directions

For the purpose of real application of a laser-produced ion beam, qualification of its characteristics, diverging both in radial and longitudinal directions as it is created from a laser-induced plasma, is a key issue. For such a purpose, we have applied radial focusing by quadrupole magnetic fields created with permanent magnets set just downstream of the production target parallel to energy focusing by an RF electric field with use of a phase rotation cavity. In Figure 3 (a), the experimental set up of the radial focusing system with the use of doublets of permanent quadrupole magnets, is shown [2]. This system can be operated with the 1Hz repetition rate using Ti:sapphire drive laser, J-KAREN, at the Kansai Photon Science Institute of the Japan Atomic Energy Agency and can focus a proton beam to a spot less than $\sim 3 \times 8 \text{ mm}^2$ at the focus spot 650 mm downstream from the production target. Using chromatic aberration of the quadrupole magnets, creation of quasi-monochromatic beam with the energy of $2.4 \pm 0.1 \text{ MeV}$ is expected from a simulation, which is supported by experimental observation with use of TOF measurement. This scheme might be one possibility to create a quasi-monoenergetic peak with attaining radial focusing, although the present method is limited in ion beam intensity and adjustability of the peak energy different from the phase rotation scheme [3]. Careful comparison between the present method and phase rotation is to be applied in quantitative manner including the capability of extension to higher ion beam energy.

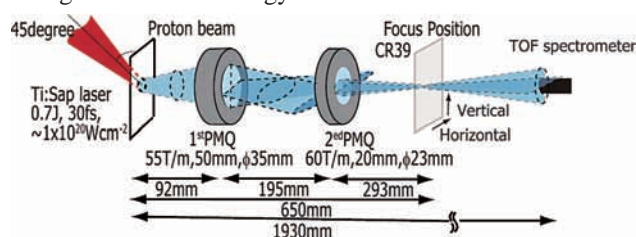


Figure 3. Experimental set up of radially focusing scheme for laser-produced protons with the use of a doublet of quadrupole magnets set just downstream of the production target.

[1] Tanabe M *et al.*: *Appl. Phys. Express*, **1**, 028001 (2008).

[2] Nishiuchi M *et al.*: *Appl. Phys. Lett.*, **94**, 061107 (2009).

[3] Nakamura S *et al.*: *Jpn. J Appl. Phys.*, **46**, L717-L720 (2007).

Award

Iwashita Y, Nishikawa Prize, "Development of an Optical Inspection System for Superconducting RF Cavities and Surface Observation", Foundation for High Energy Accelerator Science, 23 March 2009.

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

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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 T⁶-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

Research Activities (Year 2009)

Publications

Sakabe S, Hashida M, Tokita S, Namba S, Okamuro K: Mechanism for Self-Formation of Periodic Grating Structures on a Metal Surface by a Femtosecond Laser Pulse, *Phys. Rev. B*, **79**, 033409 (2009).

Nagashima T, Hirayama H, Shibuya K, Hangyo M, Hashida M, Tokita S, Sakabe S: Terahertz Pulse Radiation from Argon Clusters Irradiated with Intense Femtosecond Laser Pulses, *Optics Express*, **17**, 8907-8912 (2009).

Hashida M, Mishima H, Tokita S, Sakabe S: Non-Thermal Ablation of Expanded Polytetrafluoroethylene with an Intense Femtosecond-Pulse Laser, *Optics Express*, **17**, 13116-13121 (2009).

Sakabe S, Hashida M, Tokita S, Otani K: Laser Energy Scaling Law for the Yield of Neutrons Generated by Intense Femtosecond Laser-Cluster Interactions, *Plasma and Fusion Research*, **4**, 041 (2009).

Tokita S, Inoue S, Masuno S, Hashida M, Sakabe S: Single-Shot Ultrafast Electron Diffraction with a Laser-Accelerated Sub-MeV Electron Pulse, *Applied Physics*

Letters, **95**, 111911 (2009).

Tokita S, Murakami M, Shimizu S, Hashida M, Sakabe S: Liquid-Cooled 24 W Mid-Infrared Er:ZBLAN Fiber Laser, *Optics Letters*, **34**, 3062-3064 (2009).

Presentations

Mechanism for Self-Organization of Periodic Structures on a Metal Surface by Femtosecond Laser Pulses, Sakabe S, Hashida M, Tokita S, Namba S, Okamuro K, The European Conference on Laser and Electro-Optics 2009, Munich, Germany, 18 June 2009 (invited).

Long-Term Stabilization of Pulse-to-Pulse Energy of a High-Energy Multipass Ti:Sapphire CPA System, Tokita S, Hashida M, Masuno S, Namba S, Sakabe S, The European Conference on Laser and Electro-Optics 2009, Munich, Germany, 17 June 2009.

High Energy Ion Emission from a Copper Surface Irradiated by a Femtosecond Laser Pulse with the Laser Fluorescence of Ablation Threshold, Hashida M, Namba S, Okamuro K, Tokita S, Sakabe S, The 8th Pacific Rim Conference on

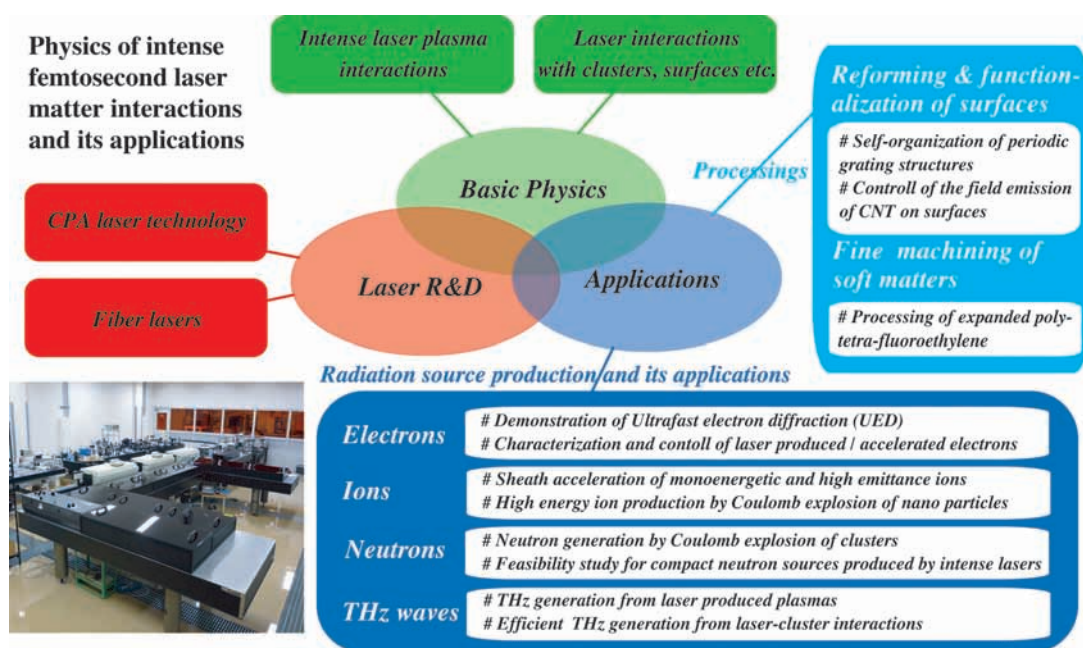
Ion Emission from Metal Surface Irradiated by Femtosecond Laser Pulses

Femtosecond laser ablation of Cu by short-pulse laser irradiation (800 nm, 130 fs) was studied in the laser energy fluence range of 0.028–14.4 J/cm². In order to elucidate the dynamics of the ejected particles, the energy distribution of ions emitted from the metal with femtosecond laser ablation was measured by time-of-flight mass spectrometry. Three thresholds for ion emission were identified. The lowest laser fluence at which ions are emitted, $F_{th,L}$ is 0.028 J/cm², and two higher emission thresholds were identified at fluences of $F_{th,M} = 0.195$ J/cm² and $F_{th,H} = 0.470$ J/cm². The number of emitted ions per laser pulse N_i was dependent on laser fluence and was in good agreement with $N_i \propto F^4$ for laser fluence of $F_{th,L} - F_{th,M}$, $N_i \propto F^3$ for laser fluence of $F_{th,M} - F_{th,H}$, and $N_i \propto F^2$ for $\geq F_{th,H}$. The process of ion production is well explained by multi-photon absorption and optical field effects. High-energy Cu ions of 30 eV were produced at a low laser fluence of 0.136 J/cm². The most probable energy of Cu ions increased as the laser energy fluence increased. The experimental results were analyzed within the framework

of the Coulomb explosion of ions that were localized to the metal surface, which could satisfactorily and qualitatively explain the obtained results.

Ultrafast Electron Diffraction with a Laser-Accelerated Electron Pulse

Ultrafast electron diffraction (UED) is a very sensitive and useful method for investigating the transient structures and dynamics of atomic and molecular systems on femtosecond to picosecond time scales. We have demonstrated single-shot measurement of electron diffraction patterns for a single-crystal gold foil using 340-keV electron pulses accelerated by intense femtosecond laser pulses with an intensity of 2×10^{18} W/cm². The measured electron beam profile is faithfully reproduced by the numerical simulation of the electron trajectory, providing evidence that the electron pulse spontaneously expands in time owing to the velocity spread produced in the acceleration process, but is not distorted in an irreversible nonlinear manner. This study shows that the laser acceleration is promising for the development of pulse compression methods for single-shot femtosecond electron diffraction.



Lasers and Electro-Optics, Shanghai, China, 31 August 2009.

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.

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 Mid-Infrared Femtosecond Fiber Laser Using Fluoride Glass Fibers, Amada Foundation for Metal Work Technology, 15 December 2008–31 March 2011.

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

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National Taiwan University, Taiwan, 1 July–30 September 2009

NanoMEGAS, Belgium, 10 September 2009

Shanghai Jiao Tong University, China, 15 September 2009

Université du Sud Toulon Var, France, 29 October 2009

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 2009)

Publications

Haruta M, Kurata H, Komatsu H, Shimakawa Y, Isoda S: Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite $\text{La}_2\text{CuSnO}_6$, *Phys.Rev.*, **B80**, 165123 (2009).

Haruta M, Kurata H, Komatsu H, Shimakawa Y, Isoda S: Effects of Electron Channeling in HAADF-STEM Intensity in $\text{La}_2\text{CuSnO}_6$, *Ultramicroscopy*, **109**, 361-367 (2009).

Yoshida K, Isoda S, Kamata T (NAIST): Epitaxial Orientation of Dimethylglyoximatoplatinum(II) on Various Substrates, *Crystal Growth & Design*, **9(6)**, 2582-2587 (2009).

Presentations

Electron Crystallography of Organic Materials by TEM, Ogawa T, Isoda S, The 26th MST Annual Conference, Chiangmai, Thailand, 28 January 2009.

Local State Analysis by Electron Energy-loss Spectroscopy in a Scanning Transmission Electron Microscope, Kurata H, NSYSU-KU Bilateral Symposium on Materials Chemistry, Kaohsiung, Taiwan, 22 September 2009.

Effects of Electron Channeling on HAADF-STEM Intensity in $\text{La}_2\text{CuSnO}_6$

Atomic resolution imaging using the high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) can be applied to analyze atomic structures of materials directly. This technique provides incoherent Z-contrast usually with the atomic number of the constituent elements. In the present work, however, unique contrasts that make intuitively interpreting the HAADF-STEM image to be difficult were observed in double perovskite oxide $\text{La}_2\text{CuSnO}_6$. Multislice simulation confirmed that this occurred as an effect of the channeling process of electrons in combination with the effect of Debye–Waller factors. This was confirmed because in the $\text{La}_2\text{CuSnO}_6$ crystal, two independent Sn atoms and four independent La atoms in the unit cell had different Debye–Waller factors, and the La columns consisted of pairs of columns with a small separation, whereas the Sn atoms were arranged straight.

Furthermore, the image contrast was examined systematically by multislice simulation on virtual structures in which two atomic La columns in the unit cell were separated by certain distances in a projected plane. As a result, the HAADF intensity did not decrease constantly

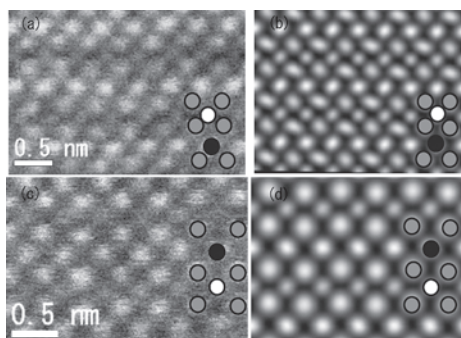


Figure 1. Experimental HAADF-STEM images of $\text{La}_2\text{CuSnO}_6$ along (a) the b-axis projection and (c) the c-axis projection. Simulated images along (b) the b-axis projection and (d) the c-axis projection.

with the increase in column separation, with the exception of a very thin sample, which could be interpreted by the specific change in the electron-channeling process.

Photochemical Synthesis of Silver Particles in Tween 20/Water/Ionic Liquid Microemulsions

Metal particles of silver (Ag) were synthesized by the photoreduction of silver perchlorate (AgClO_4) in water-in-ionic liquid (ILs: [BMIm] $[\text{BF}_4]$, [OMIm] $[\text{BF}_4]$) microemulsions consisting of Tween 20, water and ionic liquids. The time evolution of Ag particle formation by photoreduction using UV-irradiation was investigated by UV-Vis, cryo-TEM, extended X-ray absorption fine structure (EXAFS) and small angle X-ray scattering (SAXS) measurements. The average diameter of the metallic Ag particles prepared in the water-in-[BMIm] $[\text{BF}_4]$ and water-in-[OMIm] $[\text{BF}_4]$ microemulsions was estimated from TEM to be 8.9 and 4.9 nm, respectively, which was consistent with that obtained from the SAXS analysis. Using Guinier plots in a low q -range ($<0.16 \text{ nm}^{-1}$), we demonstrate that the average diameter of the water droplets that consisted of aggregates of ionic precursors of AgClO_4 before reduction and Ag particles after reduction, in the microemulsions, was estimated to be about 20–40 nm. The diameter of the water droplets increased as a function of photoreduction time because of the formation of Ag particles and their aggregates.

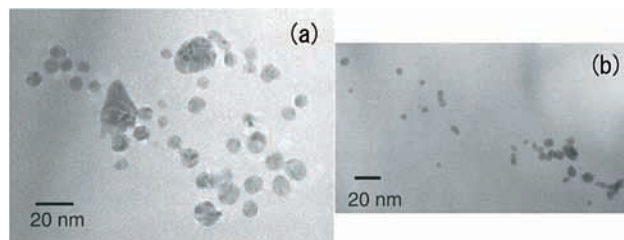


Figure 2. Cryo-TEM images of Ag particles prepared by the photoreduction in the presence of Tween 20 in (a) the water-in-[BMIm] $[\text{BF}_4]$ and (b) the water-in-[OMIm] $[\text{BF}_4]$ microemulsions.

Grants

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

mission Electron Microscope, Grant-in-Aid for Scientific Research (C) 20550188, 1 April 2008–31 March 2011.

Award

Haruta M, Kurata H, Komatsu H, Shimakawa Y, Isoda S, Best Poster Award, Site Resolved Oxygen K-edge ELNES of Layered Double Perovskites $\text{La}_2\text{CuSnO}_6$, EDGE2009: International EELS-Workshop Committee, 21 May 2009.

Advanced Research Center for Beam Science - Structural Molecular Biology -

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Scope of Research

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

Research Activities (Year 2009)

Publications

Yamauchi T, Goto M, Wu H-Y, Uo T, Yoshimura T, Mihara H, Kurihara T, Miyahara I, Hirotsu K, Esaki N: Serine Racemase with Catalytically Active Lysinoalanyl Residue, *J. Biochem.*, **145**, 421-424 (2009).

Goto M, Yamauchi T, Kamiya N, Miyahara I, Yoshimura T, Mihara H, Kurihara T, Hirotsu K, Esaki N: Crystal Structure of a Homolog of Mammalian Serine Racemase from *Schizosaccharomyces pombe*, *J. Biol. Chem.*, **284**, 25944- 25952 (2009).

Presentations

Structure of Maleylacetate Reductase from *Rhizobium* sp. strain MTP-10005, Hata Y, Fujii T, Yoshida M, Oikawa T, AsCA'09 Beijing Conference of the Asian Crystallographic Association, 23 October 2009.

Psychrophilic Tetrameric Malate Dehydrogenase Has No Intersubunit Ion-pairs, Hata Y, Fujii T, Oikawa T, Soda K, 6th Asian Biophysics Symposium, 11-12 January 2009.

Crystal Structure of GraC Involved in Resorcinol Catabolism 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 is deduced from the gene sequence.

The crystal was prepared by the sitting-drop vapour-diffusion method complemented with a microseeding technique. Good crystals were obtained at 293 K in 3 days by vapour-equilibrating drops of 1 μ l protein solution at 8 mg ml⁻¹ (in 50 mM Tris-HCl buffer, pH 8.0) and 1 μ l reservoir solution against 500 μ l 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. Diffraction data of the native crystal were collected at beamline BL6A, Photon Factory, Tsukuba, Japan with an X-ray wavelength of 1.000 Å at 100 K. The data set was collected at 1.96 Å resolution and has 44,689 independent reflections with completeness of 99.5%. The phase problem was solved with the multiwavelength anomalous diffraction method (MAD method) using the Hg-derivative crystal prepared by soaking the native crystal in the reservoir solution containing 0.025 mM ethylmercury thiosalicylate (EMTS) for 20 hours. The MAD data sets were collected at 3 Å resolution using X-rays at four wavelength-positions including the Hg-absorption edge. Each of four data sets has about 12,800 independent reflections with completeness of over 99.5%. An initial electron density map was obtained at 3 Å resolution using

MAD phases and interpreted with the help of the structure of lactaldehyde reductase (PDB ID=1RRM) which is homologous in sequence to GraC. The structure model was built by repeating the cycle of structure refinement, electron density calculation, and structure model improvement. The structure was refined at 1.96 Å resolution up to $R=0.165$ and $R_{\text{free}}=0.212$. The final structure model contains 696 of 702 amino acid residues corresponding to two polypeptide chains of GraC, 4 sulfate anions, 1 glycerol molecule, 1 benzamidine molecule and 381 water molecules.

GraC is dimeric in the crystal. Its subunit consists of two domains: the N-terminal NAD-binding domain (residues 1–159) adopting an α/β structure and the C-terminal α -helical domain (residues 160–351). The active site is located in the cleft between the domains of the subunit. The two subunits (Sub A & Sub B) have a little bit different structures from each other in the present crystal. Sub A consists of 350 residues (residues 1–350), and binds 2 sulfate anions, 1 benzamidine molecule and 1 glycerol molecule in the cleft. It has a closed conformation that may be adopted on binding the substrate with the cofactor. Sub B consists of 346 residues (residues 2–132, 134–324 and 327–350), and binds no ligand except 1 sulfate anion. It has an open conformation as is the case before the enzymatic reaction. Thus, the present crystal structure of GraC reveals the structures of maleylacetate reductase both in the substrate-binding state and in the ligand-free state. This suggests that the structure of GraC must change from the open conformation to the closed conformation in the course of enzymatic reaction.

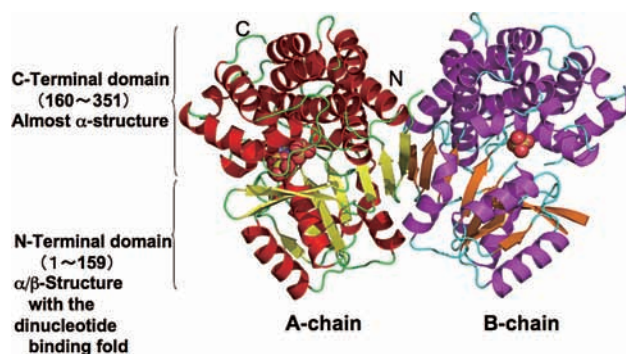


Figure 1. Structure of maleylacetate reductase (GraC) from *Rhizobium* sp. strain MTP-10005. GraC is a dimeric molecule composed of two identical subunits associating across each other.

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Dr Daisuke Hashizume	Riken, Japan, 19 June 2009
Prof Martin Kotora	Charles University, Czech Republic, 10 November 2009
Prof Petr Stepnicka	Dept. of Inorganic Chemistry, Charles University, Czech Republic, 10 November 2009
Prof Milan Pour	Dept. of Pharmacy, Charles University, Czech Republic, 10 November 2009
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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 2009)

Publications

Noda D, Sunada Y, Hatakeyama T, Nakamura M, Nagashima H: Effect of TMEDA on Iron-catalyzed Coupling Reactions of ArylMgX with Alkyl Halides, *J. Am. Chem. Soc.*, **131**, 6078-6079 (2009).

Hatakeyama T, Hashimoto S, Ishizuka K, Nakamura M: Highly Selective Biaryl Cross-Coupling Reactions between Aryl Halides and Aryl Grignard Reagents: A New Catalyst Combination of *N*-Heterocyclic Carbenes and Iron Cobalt and Nickel Fluorides, *J. Am. Chem. Soc.*, **131**,

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Ito S, Fujiwara Y, Nakamura E, Nakamura M: Iron-Catalyzed Cross-Coupling of Alkyl Sulfonates with Aryl-zinc Reagents, *Org. Lett.*, **11**, 4306-4309 (2009).

Hatakeyama T, Nakagawa N, Nakamura M: Iron-Catalyzed Negishi Coupling toward an Effective Olefin Synthesis, *Org. Lett.*, **11**, 4496-4499 (2009).

Hatakeyama T, Kondo Y, Fujiwara Y, Takaya H, Ito S, Nakamura E, Nakamura M: Iron-Catalyzed Fluoroaromatic Coupling Reactions under Catalytic Modulation with 1,2-

Iron-Group-Metal Fluoride-Catalyzed Biaryl Coupling

Combinations of *N*-heterocyclic carbenes (NHCs) and fluoride salts of the iron-group metals (Fe, Co and Ni) have been shown to be excellent catalysts for the cross-coupling reactions of aryl Grignard reagents (Ar^1MgBr) with aryl and heteroaryl halides (Ar^2X) to give unsymmetrical biaryls ($\text{Ar}^1\text{-Ar}^2$). Based on stoichiometric control experiments and theoretical studies the origin of the unique catalytic effect of the fluoride counterion can be ascribed to the formation of a higher-valent heteroleptic metalate $[\text{Ar}^1\text{M}^{\text{II}}\text{F}_2]\text{MgBr}$ as the key intermediate which undergoes oxidative addition with PhCl and releases the biaryl cross-coupling product Ph-Ph with reasonable energy barriers. The present cross-coupling reaction provides a highly selective and practical method for the synthesis of unsymmetrical biaryls as well as the opportunity to gain new mechanistic insights into the metal-catalyzed cross-coupling reactions.

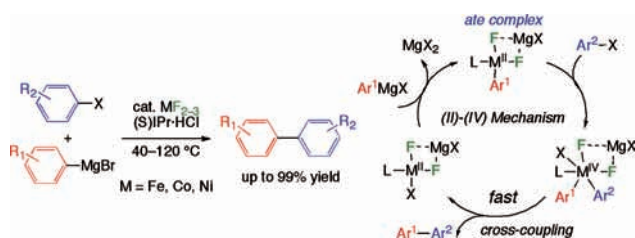


Figure 1. Selective Biaryl Coupling via (II)-(IV) Mechanism.

Iron-Catalyzed Suzuki-Miyaura Coupling

Recently iron catalysis has been intensively developed in the field of cross-coupling reaction due to its ready availability as well as high catalytic activity for the coupling of secondary alkyl halides very often superior to those of the conventional palladium and nickel catalysts. However Suzuki-Miyaura coupling among the most practical cross-coupling reaction has not been established well. We found lithium arylborate **1** prepared from arylboronic acid pinacol ester and alkyllithium can effectively cross-coupled with alkyl halides in the presence of catalytic

amount of iron (II) chloride-bisphosphine complex **2** and magnesium bromide. The features of the present method are: high-yielding chemoselective and free of rare metals showing its potential in efficient and versatile access to functional aromatic compounds.

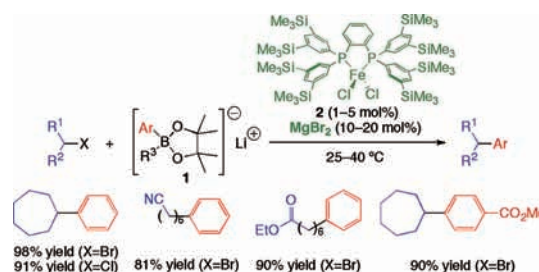


Figure 2. Suzuki-Miyaura Coupling of Alkyl Halides with Arylborates.

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 photochemical devices advanced catalysts artificial enzymes and MRI contrast agents will be explored with a diverse library of metallated-amino acids and peptides.

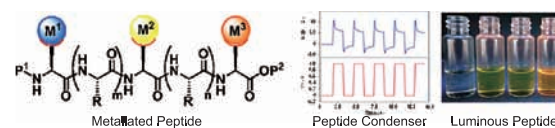


Figure 3. Preparation of Metallated Peptide and Self-Assembly of the Peptide.

Bis(diphenylphosphino)benzene, *Chem. Commun.*, 1216-1218 (2009).

Presentations

Selective Cross-Coupling Reactions Based on Iron Catalyst, Nakamura M, Summer Symposium The Japanese Society for Process Chemistry, 16-17 July 2009, Chiba, Japan (invited).

Iron-Catalyzed Suzuki-Miyaura Coupling Reaction, Nakamura M, The 14th Japan-Korea Symposium on Organic Chemistry, 23-26 October 2009, Atami, Japan (invited).

Selective Cross-Coupling Reactions Based on Iron and Iron-Group Metal Catalysts, Nakamura M, Japan Petroleum Institute Catalyst Symposium, 24 November 2009, Tokyo, Japan (invited).

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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 2009)

Publications

Long YW, Hayashi N, Saito T, Azuma M, Muranaka S, Shimakawa Y: Temperature-induced A-B Intersite Charge Transfer in an A-site-ordered $\text{LaCu}_3\text{Fe}_4\text{O}_{12}$ Perovskite, *Nature*, **458**, 60-63 (2009).

Kawai M, Ito K, Shimakawa Y: Resistance Switching in a Single-crystalline NiO Thin Film Grown on a $\text{Pt}_{0.8}\text{Ir}_{0.2}$ Electrode, *Applied Physics Letters*, **95**, [012109-1]-[012109-3] (2009).

Presentations

New Perovskite-type Structure Oxides: High-pressure Synthesized Bulks and Epitaxially Grown Thin Films: Shimakawa Y, Gordon Research Conferences, Solid State Chemistry, Oxford, UK, 2 September 2009.

Ferromagnetic Cuprates $\text{CaCu}_3\text{B}_4\text{O}_{12}$ ($B = \text{Ge, Sn}$) Synthesized under High Pressure: Saito T, International Conference on High Pressure Science and Technology, Tokyo, Japan, 31 July 2009.

Frustrated $S=3/2$ Honeycomb Antiferromagnet $\text{Bi}_3\text{Mn}_4\text{O}_{12}(\text{NO}_3)$: Azuma M, International Conference on Magnetism, Superconductivity and Phase Transitions in Novel and Complex Materials 2009, Kolkata, India, 12 November 2009.

Grant

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.

Temperature-Induced A–B Intersite Charge Transfer in an A-Site-Ordered LaCu₃Fe₄O₁₂ Perovskite

Changes of valence states in transition-metal oxides often cause significant changes in their structural and physical properties. Chemical doping is the conventional way of modulating these valence states. In ABO₃ perovskite and/or perovskite-like oxides, chemical doping at the A site can introduce holes or electrons at the B site, giving rise to exotic physical properties like high-*T_c* superconductivity and colossal magnetoresistance. When valence-variable transition metals at two different atomic sites are involved simultaneously, we expect to be able to induce charge transfer -and, hence, valence changes- by using a small external stimulus rather than by introducing a doping element. Materials showing this type of charge transfer are very rare, however, and such externally induced valence changes have been observed only under extreme conditions like high pressure. We found unusual temperature-induced valence changes at the A and B sites in the A-site-ordered double perovskite LaCu₃Fe₄O₁₂ (Figure 1); the underlying intersite charge transfer is accompanied by considerable changes in the material's structural, magnetic and transport properties. When cooled, the compound shows a first-order, reversible transition at 393K from LaCu²⁺₃Fe^{3.75+}₄O₁₂ with Fe^{3.75+} ions at the B site to LaCu³⁺₃Fe³⁺₄O₁₂ with rare Cu³⁺ ions at the A site. Intersite charge transfer between the A-site Cu and B-site Fe ions leads to paramagnetism-to-antiferromagnetism and metal-to-insulator isostructural phase transitions. What is more interesting in relation to technological applications is that this above-room-temperature transition is associated with a large negative thermal expansion.

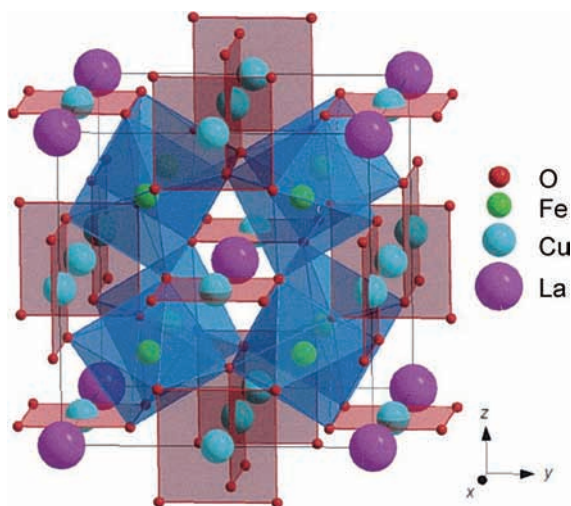


Figure 1. Crystal structure of LaCu₃Fe₄O₁₂

Resistance Switching in a Single-Crystalline NiO Thin Film Grown on a Pt_{0.8}Ir_{0.2} Electrode

Resistance switching (RS) phenomena in an M/NiO/M (M: Metal) capacitor structure, where a thin film of NiO is sandwiched between two metal electrode layers, have attracted much attention because of their potential applications for resistive random access memories. The RS in a polycrystalline NiO thin film has been explained by a filamentary conducting path mechanism, in which formation and rupture of the conducting filaments in the oxide layer. However, the properties also affected by grain and/or domain boundaries in the polycrystalline sample. In order to see the “intrinsic” behaviors of filaments, investigations of RS properties in a single-crystalline NiO thin film are needed. We recently succeeded in preparing Pt/NiO/Pt-Ir with a single-crystalline NiO thin film on an atomically flat Pt-Ir epitaxial bottom electrode layer (Figure 2). The memory cells showed unipolar resistance switching behaviors (Figure 3). The result demonstrates that unipolar resistance switching is not a characteristic phenomenon in the polycrystalline NiO but it can also occur in the single-crystalline NiO.

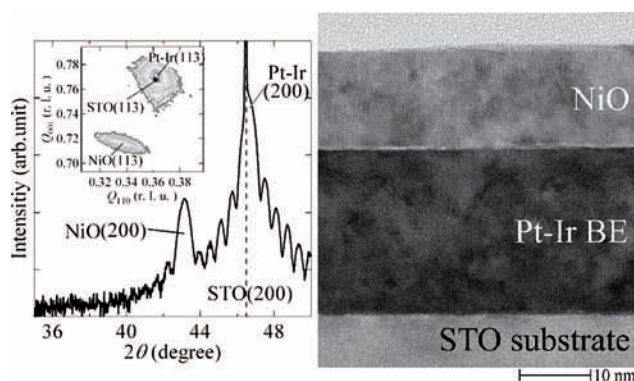


Figure 2. X-ray diffraction profiles and a cross-sectional TEM image of a Pt/NiO/Pt-Ir capacitor structure.

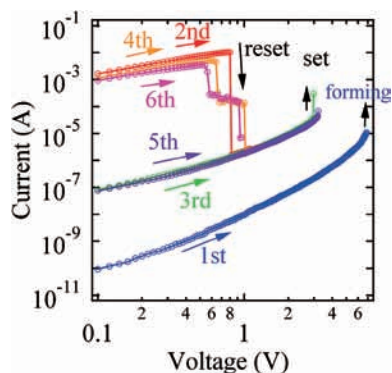


Figure 3. RS behaviors observed in an Pt/NiO/Pt-Ir capacitor.

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Scope of Research

This laboratory aims at establishment of new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using experimental methods such as 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 2009)

Publications

Wakioka M, Nakajima Y, Ozawa F: Mechanism of C-P Reductive Elimination from *trans*-[Pd(CH=CHPh)Br(PMePh₂)₂], *Organometallics*, **28**, 2527-2534 (2009).

Wakioka M, Mutoh Y, Takita R, Ozawa F: A highly Selective Catalytic System for the Cross-Coupling of (*E*)-Styryl Bromide with Benzeneboronic Acid: Application to the Synthesis of All-Trans Poly(arylenevinylene)s, *Bull. Chem. Soc. Jpn.*, **82**, 1292-1298 (2009).

Okazaki M, Takano M, Ozawa F: Redox-responsive Recombination of Carbon-Carbon Bonds on Flexible Tetrairon Cores, *J. Am. Chem. Soc.*, **131**, 1684-1685 (2009).

Presentations

Synthesis and Properties of Bis(phosphaethenyl)pyridine Iron Complexes, Ozawa F, Nakajima Y, The 14th Japan-Korea Joint Symposium on Organometallic and Coordination Chemistry, 9 October 2009, Nagoya, Japan (Invited).

Synthesis and Properties of All-cis Poly(arylene vinylene)₂, Ozawa F, Takita R, NSYU-KU Bilateral Symposium on Materials Chemistry, 23 September 2009, Kaohsiung, Taiwan.

Grants

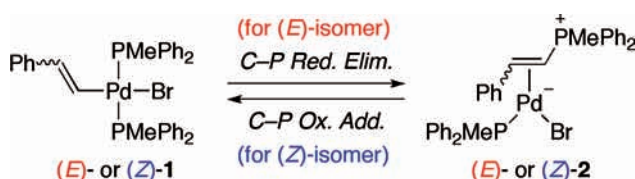
Ozawa F, Okazaki M, Takita R, Nakajima Y, Synergistic Effects of Transition Metals and Heavier Main Group Elements in Functional Organometallic Complexes, Grant-in-Aid for Priority Area "Synergy of Elements", 1 September 2006–31 March 2010.

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

Mechanism of C-P Reductive Elimination from *trans*-[Pd(CH=CHPh)Br(PMePh₂)₂]

While the C-P reductive elimination of hydrocarbyl and phosphine ligands are frequently observed in catalytic processes promoted by palladium phosphine complexes, its mechanistic information has been limited. In this work, we prepared the (*E*)- and (*Z*)-styryl isomers of *trans*-[Pd(CH=CHPh)Br(PMePh₂)₂] (**1**) and [Pd(η^2 -PhCH=CHPMePh₂)Br(PMePh₂)] (**2**), and examined their C-P reductive elimination (**1** \rightarrow **2**) and C-P oxidative addition (**2** \rightarrow **1**) behaviors. Kinetics and thermodynamics of the reactions are strongly affected by *E/Z* configurations of the styryl group and solvent polarity. The (*E*)-isomer of **1** undergoes C-P reductive elimination easily in polar CD₂Cl₂ to afford (*E*)-**2** in high selectivity, whereas C-P oxidative addition of (*Z*)-**2** giving (*Z*)-**1** takes place favorably in non-polar C₆D₆. X-Ray diffraction analysis and DFT calculations for **1** and **2** provided reasonable accounts for these reaction features. Kinetic examinations revealed two types of C-P reductive elimination processes, which involve pre-dissociation and association of PMePh₂ ligand, respectively.

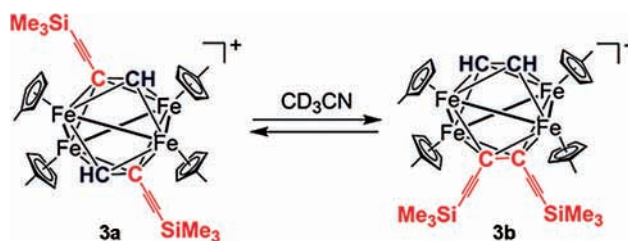


Scheme 1. C-P reductive elimination and oxidative addition behaviors of complexes **1** and **2**.

Redox-Responsive Recombination of Carbon-Carbon Bonds on Flexible Tetrairon Cores

Although there have been many studies on tetranuclear transition metal clusters, the interconversion between each cluster core structure remains poorly understood. Based on these facts, we investigated the geometry interconversion of the tetrairon core using [$(\eta^5$ -C₅H₄Me)₄Fe₄(Me₃SiCCH)₂] (PF₆) (**3a**) as a probe. When a brown powder of **3a** was dissolved in acetonitrile, **3a** was converted to **3b**. Equilibrium was reached at a 74:26 molar ratio within 1 week at 303

K. The isomerization proceeds through a cubane-like transition state, in which recombination of a carbon-carbon bond occurs.



Scheme 2. Recombination of carbon-carbon bonds on tetrairon cores.

The Effects of Primary Structures on Photo-induced Insolubilization of All-cis Poly(*p*-phenylenevinylene)s in Thin Films

All-cis PPVs prepared by Suzuki-Miyaura-type polycondensation undergo photo-induced insolubilization in thin films, along with cis-to-trans isomerization of vinylene linkages to give all-trans PPVs. This phenomenon has been investigated in detail, using all-cis and all-trans PPVs with a range of molecular weights and terminal structures. It has been found that the all-cis configuration serves as a particularly important factor.

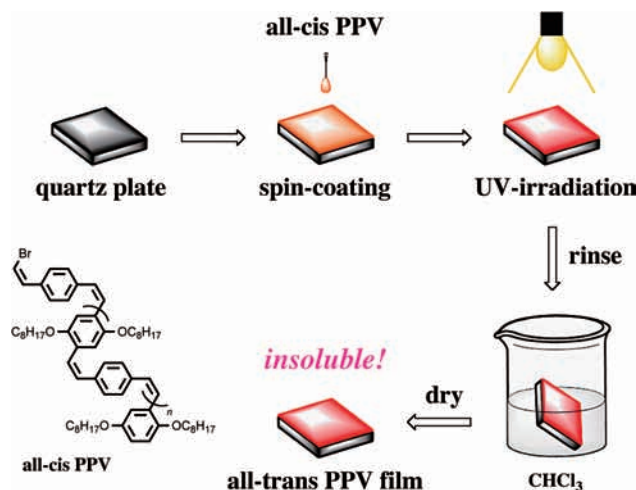


Figure 1. Photo-induced insolubilization of all-cis poly(*p*-phenylenevinylene)s in thin films.

Takita R, Development of Efficient Synthetic Methodologies Based on Direct Functionalization Reactions, Grant-in-Aid for Young Scientists (B), 1 April 2009–31 March 2011.

Nakajima Y, Efficient Photoreduction of Carbon Dioxide Catalyzed by an Iron Complex Bearing a Phosphaalkene Ligand, PRESTO Program, Japan Science and Technology Agency, 1 October 2009–31 March 2012.

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Scope of Research

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

Research Activities (Year 2009)

Publications

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

Matsunaga R, Miyauchi Y, Matsuda K, Kanemitsu Y: Symmetry-induced Nonequilibrium Distributions of Bright and Dark Exciton States in Single Carbon Nanotubes, *Phys. Rev. B*, **80**, [115436-1]-[115436-6] (2009).

Miyauchi Y, Hirori H, Matsuda K, Kanemitsu Y: Radiative Lifetimes and Coherence Lengths of One-dimensional Excitons in Single-walled Carbon Nanotubes, *Phys. Rev. B*, **80**, [081410(R)-1]-[081410(R)-4] (2009).

Tayagaki T, Fukatsu S, Kanemitsu Y: Photoluminescence Dynamics and Reduced Auger Recombination in Si_{1-x}Ge_x/Si Superlattices under High-density Photoexcitation, *Phys. Rev. B*, **77**, [041301(R)-1]-[041301(R)-4] (2009).

Presentations

Exciton Radiative Lifetimes and Their Temperature Dependence in Single-Walled Carbon Nanotubes, Miyauchi Y, Matsunaga R, Hirori H, Matsuda KT, Kanemitsu Y, 2009 APS March Meeting, 16–20 March 2009, Pittsburgh, USA.

Luminescence and Magnetic Properties of Co Doped ZnO Nanocrystals, Taguchi S, Tayagaki T, Kanemitsu Y, European Materials Research Society (E-MRS), 8–12 June 2008, Strasbourg, France.

Exciton Fine Structures and Dynamics Studied by Single Carbon Nanotube Spectroscopy, Matsuda K, 3rd Workshop on Nanotube Optics & Nanospectroscopy (WONTON'09), 7–10 June 2009, Sendai, Japan.

Quantized Auger Recombination and Carrier Multiplication in Semiconductor Nanoparticles and Carbon Nanotubes, Kanemitsu Y, Ueda A, Tayagaki T, Matsuda K, 23rd International Conference on Amorphous and Nanocrystalline Semiconductors (ICANS 23), 23–28 August 2009, Utrecht, Netherlands.

Grants

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

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

Temperature Dependence of Photoluminescence Spectra of Nondoped and Electron-doped SrTiO₃: Crossover from Auger Recombination to Single-carrier Trapping

Transition metal oxides have attracted a great deal of attention as new device materials due to their wide variety of fascinating and multifunctional properties. SrTiO₃ is one of the most important oxide materials. We studied photoluminescence (PL) decay dynamics in highly photo-excited SrTiO₃ crystals at low temperatures. The PL spectrum and dynamics show abrupt changes below 150 K in both nondoped and electron-doped SrTiO₃ samples. We clarified that the PL dynamics in both nondoped and electron-doped SrTiO₃ is well described by the same simple model involving single-carrier trapping, radiative bimolecular recombination, and nonradiative Auger recombination. The unusual temperature dependence of PL dynamics is caused by the crossover from Auger recombination at high temperatures to single-carrier trapping at low temperatures.

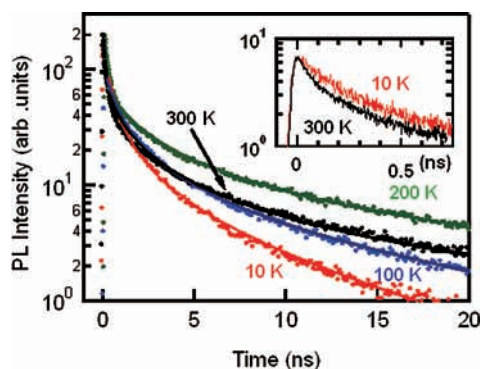


Figure 1. Temperature dependence of PL decay curves of nondoped SrTiO₃. Inset: PL decay profiles in the sub-nanosecond region.

Mn-Mn Couplings in Mn-doped CdS Nanocrystals Studied by Magnetic Circular Dichroism Spectroscopy

Fabrication and characterization of semiconductor nanocrystals (NCs) doped with functional impurities have been extensively studied due to interest both in the fundamental physics and potential applications in optoelectronic devices. We studied on the optical and magnetic properties of Mn-doped CdS nanocrystals coated with a ZnS shell

layer (CdS:Mn/ZnS core-shell nanocrystals) by magnetic circular dichroism (MCD) spectroscopy. The magnetic field and temperature dependences of the MCD spectrum show paramagnetic behavior of the CdS:Mn/ZnS core-shell nanocrystals. The MCD intensity increases with the Mn concentration up to a few mol-%, and then starts to decrease rapidly. This Mn-concentration dependence of the MCD intensity can be explained by the formation of Mn-Mn pairs in heavily doped nanocrystals.

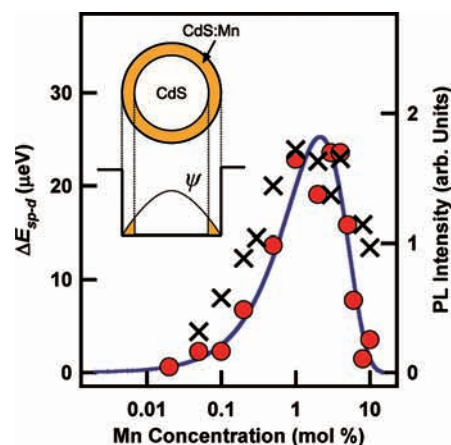


Figure 2. The splitting energy due to *sp-d* exchange (circles) and PL intensities (crosses) of Mn-doped CdS NCs as a function of the Mn concentration. Inset: Schematic illustration of model Mn-doped CdS NC.

Photoluminescence Dynamics and Reduced Auger Recombination in Si_{1-x}Ge_x/Si Superlattices under High-density Photoexcitation

Electronic and optical properties in various types of Si nanostructure have been extensively studied both from the viewpoint of fundamental physics and the potential application to electronic and optical devices. We studied PL dynamics and multi-exciton recombination in Si_{1-x}Ge_x/Si superlattices under high-density excitation. Saturation of the PL intensity and rapid PL decay are observed as the excitation laser intensity is increased. These phenomena occur due to nonradiative Auger recombination of the electron-hole pairs. The Auger process in Si_{1-x}Ge_x/Si superlattices is less pronounced than that in the Si_{1-x}Ge_x/Si single quantum wells. Our findings show that coupled nanostructures have an advantage in efficient light emission and the control of many-body carrier dynamics.

Bioinformatics Center - Bioknowledge Systems -

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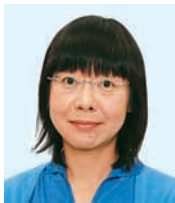
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Scope of Research

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 information 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 2009)

Grants

Kanehisa M, Backbone Database for Analysis of the Biological Systems and Environment, Grants-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.

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

E-zyme: Predicting Potential EC Numbers from the Putative Enzyme Reactions

The high-throughput screenings of biochemical compound libraries have been producing huge amounts of chemical data, and we are now confronted with the necessity to automate the processing and interpretation of such chemical data in order to derive biologically meaningful information. There are numerous enzyme reactions known to be present in various metabolic pathways but without any official EC (Enzyme Commission) numbers, most of which have no hope to be given ones because of the lack of the published articles on enzyme assays.

We have been developing a new method to predict an EC sub-subclass based on our original biochemical transformation pattern which we call an "RDM pattern", and develop a web-server called "E-zyme" which enables us to automatically assign the potential EC numbers to given pairs of substrates and products, or uncharacterized reactions. The original version of the E-zyme was established in 2004 (Kotera et al., *J. Am. Chem. Soc.*, 2004, **126**(50): 16487-16498), and we published the latest version with improved coverage, recall and precision in 2009 (Yamanishi et al., *Bioinformatics*, 2009, **25**(12): i179-i186). The E-zyme system can provide a link to the corresponding enzyme candidate genes. The next possible development involves specifying which genes are actually involved in the reaction of interest for a specific organism.

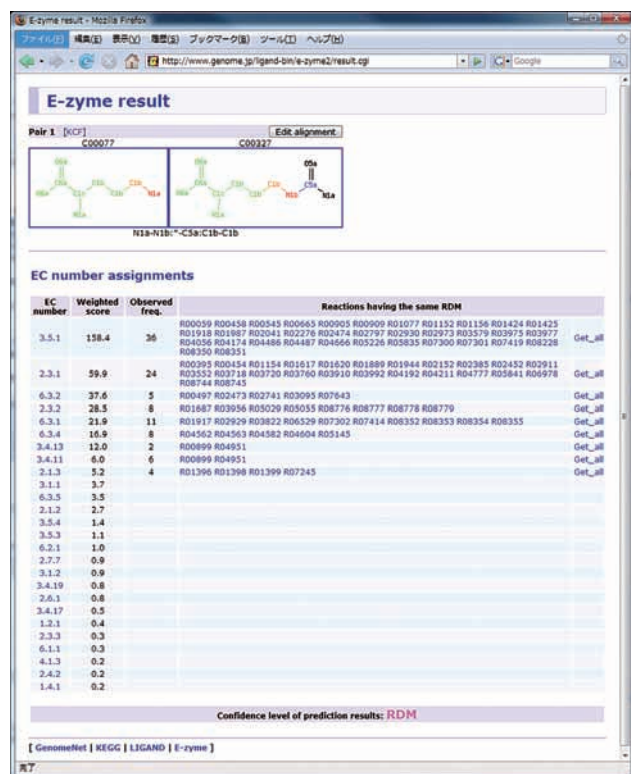


Figure 1. A screenshot of the E-zyme output page.

varDB: a Database for Studying Antigenic Variation

Antigenic variation plays a major role in immune evasion and establishment of persistent infections for many pathogens, including HIV (AIDS), *Plasmodium falciparum* (malaria), etc. Due to the inherent complexities associated with multi-gene families, antigenic variation studies are usually focused on single gene families and restricted to a small number of organisms. To lessen these limitations and promote cross-species and comparative genomic studies, we have developed varDB. VarDB is a public resource that collects genes and proteins from known antigenic variant gene families. The main goals of the varDB project are: I) to serve as a repository for antigenic variant gene families, II) to work as a platform for the analysis of antigenic variation between different organisms, and III) to be a community driven resource enabling synergistic cooperation from experts in different antigenic gene families. As of October 2009, the varDB project contains sequence data of 49 gene families, from 31 different pathogens that cause 22 diseases. Together, more than 68,000 sequences are available, including those obtained from clinical samples around the world. The database is expected to expand in the future as new sequences are being submitted to repositories like GenBank, and more antigenic variant gene families are identified. Many different tools for sequence analysis are integrated, providing a unique framework for cross-species analysis.

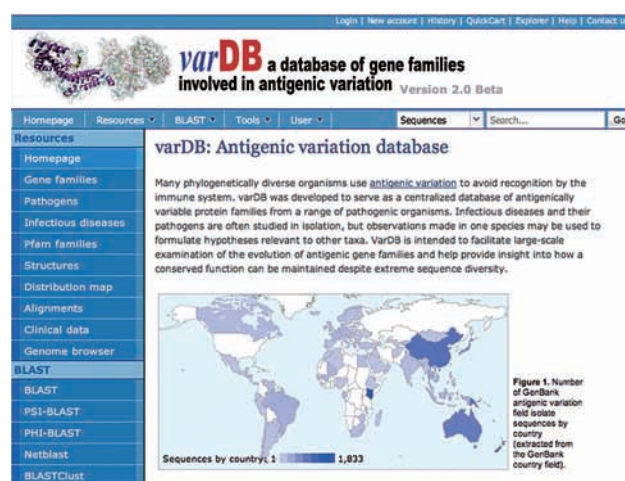


Figure 2. Home page of the varDB project, showing in the left panel the resources and part of the available tools. The map indicates the location and density of antigenic variant sequences collected in the database.

Bioinformatics Center - Biological Information Networks -

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



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CONG, Yang The University of Hong Kong, China, 7 May–4 August 2009
Dr VERT, Jean-Philippe Mines ParisTech and Curie Institute, France, 19 June–18 August 2009
Dr MELKMAN, Avraham Ben Gurion University, State of Israel, 14 October 2009–5 January 2010

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 2009)

Publications

Nacher JC, Hayashida M, Akutsu T: Emergence of Scale-Free Distribution in Protein-Protein Interaction Networks Based on Random Selection of Interacting Domain Pairs, *BioSystems*, **95**, 155-159 (2009).

Tamura T, Akutsu T: Algorithms for Singleton Attractor Detection in Planar and Nonplanar AND/OR Boolean Networks, *Mathematics in Computer Science*, **2**, 401-420 (2009).

Kato Y, Akutsu T, Seki H: Dynamic Programming Algorithms and Grammatical Modeling for Protein Beta-Sheet Prediction, *Journal of Computational Biology*, **16**, 945-957 (2009).

Presentations

Comparing Biological Networks via Graph Compression, Hayashida M, 3rd International Symposium on Optimization and Systems Biology (OSB 2009), 20 September 2009.

Completing Networks Using Observed Data, Tamura T, 20th International Conference on Algorithmic Learning

Theory (ALT 2009), 4 October 2009.

Integer Programming-Based Methods for Attractor Detection and Control of Boolean Networks, Akutsu T, The combined 48th IEEE Conference on Decision and Control and 28th Chinese Control Conference (IEEE CDC 2009), 17 December 2009.

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 2010.

Finding Minimum Reaction Cuts of Metabolic Networks under a Boolean Model Using Integer Programming and Feedback Vertex Sets

In this work, we consider the problem of, given a metabolic network, a set of source compounds and a set of target compounds, finding a minimum size reaction cut, where a Boolean model is used as a model of metabolic networks. The problem has potential applications to measurement of structural robustness of metabolic networks and detection of drug targets. We develop an integer programming based method for this optimization problem. In order to cope with cycles and reversible reactions, we further develop a novel integer programming (IP) formalization method using a feedback vertex set (FVS). When applied to an *E. coli* metabolic network consisting of Glycolysis/Glyconeogenesis, Citrate cycle and Pentose phosphate pathway obtained from KEGG database, the FVS-based method can find an optimal set of reactions to be inactivated much faster than a naive IP-based method and several times faster than a flux balance-based method. We also confirm that our proposed method works even for large networks and discuss the biological meaning of our results.

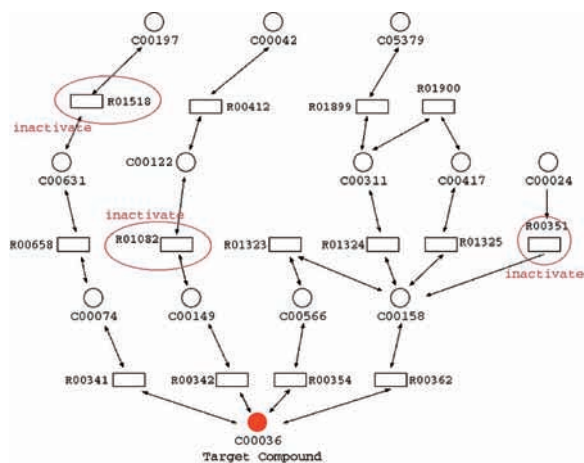


Figure 1. Relationship among the target compound and deleted reactions when C00036 is the target compound. In our computer experiment with a partial map of KEGG, deleting {R00351, R01082, R01518} effectively prevented the target compound to be produced.

Comparing Biological Networks via Graph Compression

One of the central problems in bioinformatics and systems biology is comparison of various kinds of biological data. Methods for comparison of DNA and/or protein sequences have been extensively studied and have been applied to analyses of real sequence data quite successfully. On the other hand, data compression methods have been applied to comparison of large sequence

data and protein structure data. Since it is still difficult to compare global structures of large biological networks and data compression-based methods can be applied to comparison of large-scale sequence data, it is reasonable to try to apply data compression methods to comparison of biological networks.

Here, we propose a novel method for comparing biological networks. In the proposed method, an original network structure is compressed by iteratively contracting identical edges. Then, the similarity of two networks is measured by a compression ratio of the concatenated networks. The proposed method is applied to comparison of metabolic networks of *H. sapiens*, *M. musculus*, *A. thaliana*, *D. melanogaster*, *C. elegans*, *E. coli*, *S. cerevisiae*, and *B. subtilis*. The results suggest that our method can efficiently measure the similarities between metabolic networks.

Hayashida M, Akutsu T: *Lecture Notes in Operations Research*, pp. 168-176.

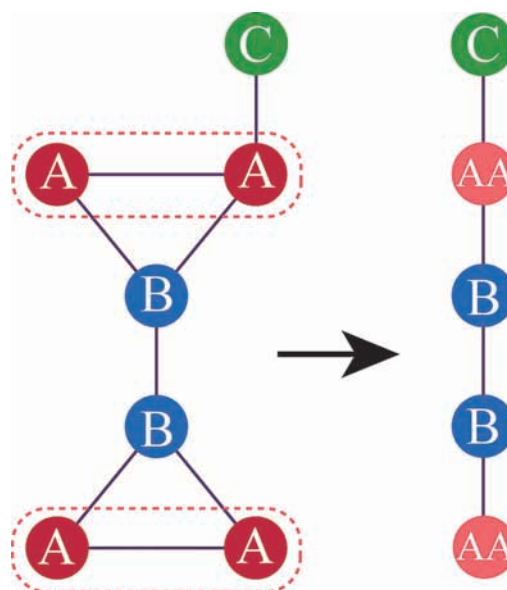


Figure 2. Example of edge contraction.

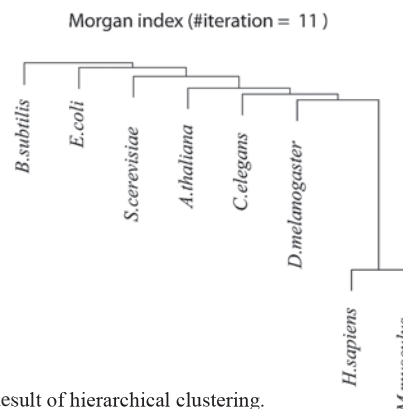


Figure 3. Result of hierarchical clustering.

Bioinformatics Center - Pathway Engineering -

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



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du VERLE, David

Inserm, France, 1 February–17 March 2009

NGUYEN, Hao Canh

JAIST, Japan, 23 February 2009

Dr NG, See-Kiong

A*Star, Singapore, 16–23 April 2009

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 2009)

Publication

Kayano M, Takigawa I, Shiga M, Tsuda K, Mamitsuka H: Efficiently Finding Genome-wide Three-way Gene Interactions from Transcript- and Genotype-Data, *Bioinformatics*, **25 (21)**, 2735-2743 (2009).

Presentations

Mining Significant Patterns from Trees, Mamitsuka H, Université Louis Pasteur, Strasbourg, France, 28 May 2009.

Clustering with Heterogeneous Data, Mamitsuka H, IEEE International Conference on Computational Intelligence and Natural Computing (CINC 2009), Wuhan,

China, 6 June 2009.

A Markov Classification Model for Metabolic Pathways, Mamitsuka H, Fudan University, Shanghai, China, 29 September 2009.

Mining Significant Patterns from Glycan Structures, Mamitsuka H, International Beilstein Symposium on Glyco-Bioinformatics, Potsdam, Germany, 5 October 2009.

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

Efficiently Finding Genome-wide Three-way Gene Interactions from Transcript- and Genotype-Data

The topical work this year is the issue of finding a three-way gene interaction, precisely two interacting genes in expression under the genotypes of a different gene, given a dataset in which both gene expressions and genotypes are measured for each individual. We illustrate our problem setting by using synthetic 2D diagrams in Figure 1, where expression values of two genes are plotted with three classes (genotypes): +, * and Δ. In this figure, (a) shows expression values being just randomly distributed; (b) shows expression values being easily categorized into three classes; and (c) shows that classes can be categorized by expressions without using two genes at the same time. We are not interested in (a–c) but in (d), which shows that the correlation in expression between two genes differs for each class. More concretely, two genes are positively correlated for one class, whereas they are negatively correlated for another. This is exactly a switching mechanism in expression between correlation and inverse-correlation of two genes, controlled by another gene. At the same time, this is the three-way gene interaction which we are interested in. We emphasize that this interaction is key to elucidating complex biological systems.

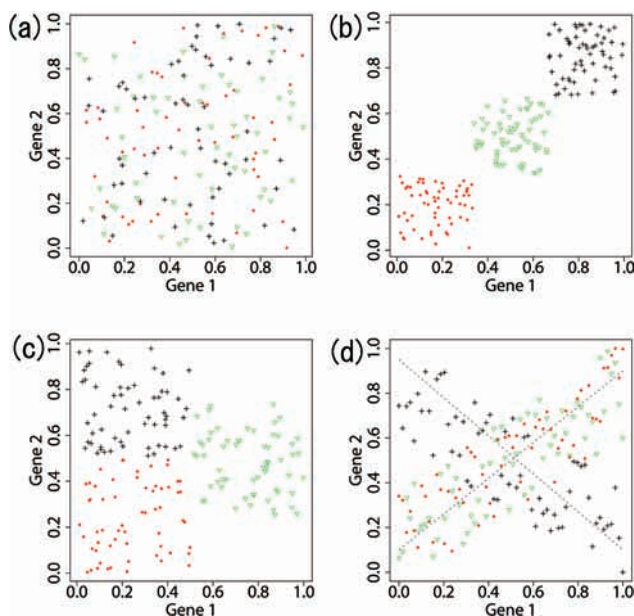


Figure 1.

A usual, common approach to detect the three-way interaction is the likelihood ratio test for regression. Particularly, logistic regression must be suitable the most, because of categorical responses (genotypes) in our setting. However, parameter estimation for logistic regression is based on the maximum likelihood, for which only a time-consuming iterative gradient descent, Newton–Raphson, is usually used. In our case, classes are genotypes, resulting in a problem of an explosive number of combinations of one SNP (genotypes) and two genes (expressions). For example, for 50,000 SNPs and 1,000 genes, we have roughly 5×10^{10} ($= 50,000 \times 1,000 \times 1,000$) combinations, making scanning over all possible combinations intractable. Thus, the main focus of this work is to speed up the procedure of finding the three-way interactions. Our strategy for this issue is to prune irrelevant combinations, such as those in which the expression values of two genes are randomly distributed as in Figure 1(a), by using statistical testing assuming the normality of given examples. Our experiments with a huge dataset of human brain samples showed that our method 1) run 10 times faster than likelihood ratio test with logistic regression for any data size, keeping the accuracy of detecting three-way interactions at around 85% and 2) detected a large number of three-way gene interactions we were looking for. Figure 2 shows a typical example of the detected interactions with p -value of -8.91 , where two genes are correlated with each other under two classes or anti-correlated under the other class. We confirmed the plausibility of this interaction in terms of the biological literature.

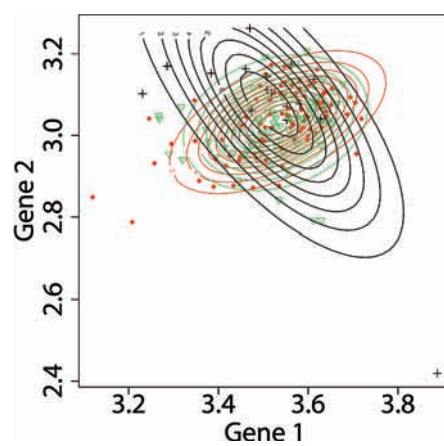


Figure 2.

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.

Endowed Research Section - Water Chemistry Energy (AGC) -

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



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TSUJINO, Yasuo

Researcher

TANAKA, Toshiyuki

Visitor

Prof ROSSKY, Peter J. University of Texas at Austin, USA, 25–29 June 2009

Scope of Research

Application of fundamental studies on decomposition and formation of formic acid to the hydrogen energy technology is under investigation using NMR, Raman, and IR spectroscopy. This hydrogen-water energy cycle with formic acid does make a contribution to the CO₂ reduction and to a progress in energy-saving society. We are taking advantage of the solvation effect on the equilibrium of formic acid formation or decomposition from formic acid to capture and deposit CO₂ on a large scale.

Research Activities (Year 2009)

Publications

Yoshida K, Matubayasi N, Nakahara M: Self-diffusion Coefficients for Water and Organic Solvents in Extremely Low-density Supercritical States, *J. Mol. Liq.*, **147**, 96-101, 2009.

Yasaka Y, Wakai C, Matubayasi N, Nakahara M: Water as an In-situ NMR Indicator for Acid Impurities in Ionic Liquids, *Anal. Chem.*, **81**, 400-407, 2009.

Presentations

Supercritical Water from the Viewpoint of Nanoscience, Nakahara M, The 1st Symposium on Center for Nanoscience Research, Kyoto, 7 March 2009.

Solution Chemistry Today and Future Perspectives, Nakahara M, The 76th Conference on the Electrochemical Society of Japan, Kyoto, 31 March 2009.

The Old Man and the Chemistry, Nakahara M, Workshop on the Future of Solution Chemistry, Kyoto, 27 June 2009.

Hydrothermal Chemistry of Formic Acid and New Scheme of Hydrogen Technology, Nakahara M, Yoshida K, Yasaka Y, Tsujino Y, Wakai C, Matubayasi N, International Conference on High Pressure Science and Technology (Joint AIRAPT-22 & HPCJ-50), Tokyo, 31 July 2009.

Formic Acid as a Chemical Tank for Hydrogen, Nakahara M, The International Association for the Properties of Water and Steam, Netherlands, 8 September 2009.

Grant

Nakahara M, Development of Formic Acid Production Highly Controlled by the Water-Gas Shift Reaction, Aiming at the Hydrogen Storage and the Hydrogen Transportation, to Promote Basic Research by Research Personnel in Private-Sector Business, Japan Science and Technology Agency, 1 December 2009–30 November 2010.

The Hydrogen-Water Energy Cycle with Formic Acid as a Chemical Tank for Hydrogen

Water is potentially a useful medium for organic chemical reactions. At room temperature, however, the utility of water as a reaction medium is restricted by the low solubility of organic compounds. Super- and subcritical water is a promising medium to overcome this restriction. When the temperature is elevated, water mixes well with organic compounds, including such nonpolar gases as H₂, CO, and CO₂. The hydrogen bonding persists in hot water, and the modified water-gas-shift (WGS) reaction,



can be controlled in hot water to develop the hydrogen-water-energy cycle technology. Our mission is to develop the earth-friendly technology using the new WGS reaction mentioned above. The new WGS reaction has the potential to store and transport hydrogen safely and to reduce the green-house gas CO₂ emission that may induce some

climate changes. Hydrogen is an ultimately clean fuel compared with fossil fuels; CO₂ emission per energy from hydrogen is the lowest and is recyclable energy from H₂O and CO. However, the drawback of the hydrogen fuel arises from the low liquefaction temperature. This results in a high cost and delays the realization of the clean hydrogen age. Fuel compactness and fluidity, as attained in the liquid state, are necessary for the low-cost transportation and storage. This can be overcome by taking advantage of formic acid that is found as an intermediate in the water-gas shift reaction. CO₂ can be fixed to formic acid by utilizing surplus hydrogen which is discharged by a plant such as the soda plant and the iron work. The hydrogen-water-energy-cycle technology with the formic acid intermediate can realize both the new clean energy cycle and the low CO₂ emission, as shown in Figure 1.

On the basis of the kinetics and equilibrium of the formic acid decomposition, the new WGS reaction can be controlled in a desirable direction by tuning temperature and pressure of hot water or ionic liquids. The application of the new WGS reaction for hydrogen energy production and storage is thus hopeful in the future.

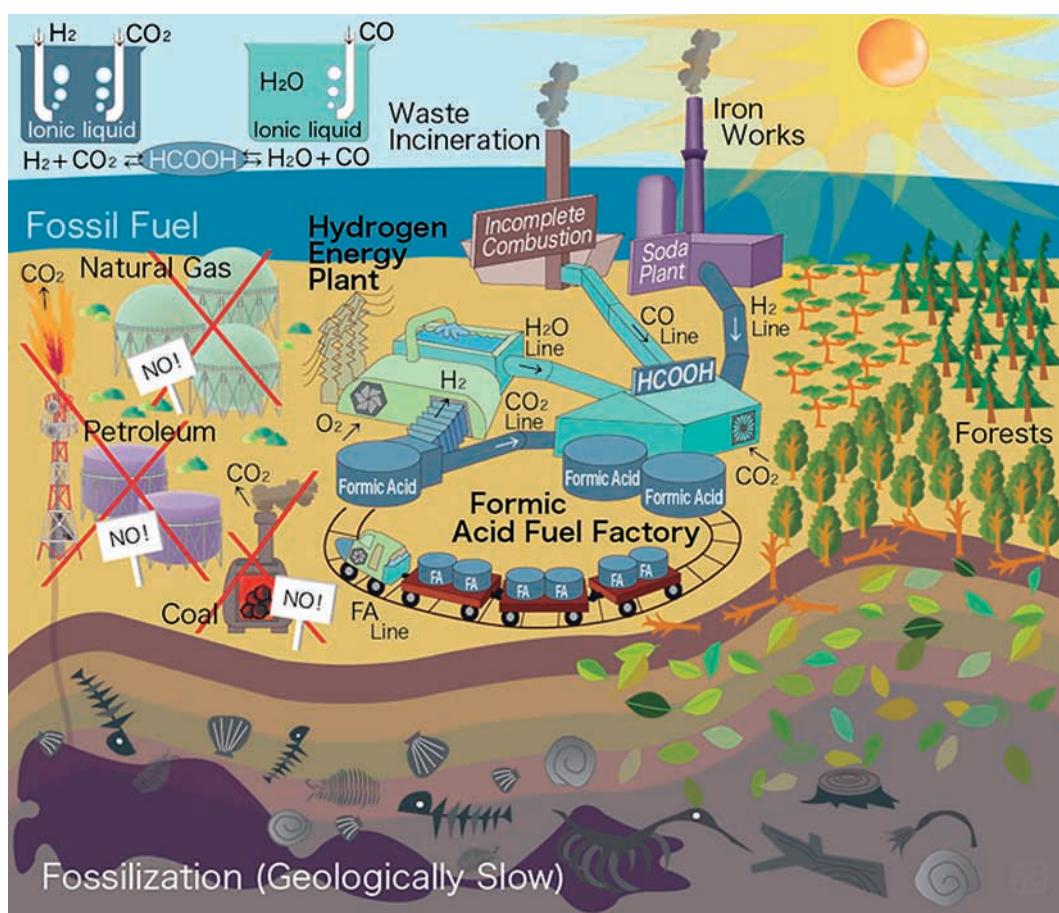


Figure 1. The hydrogen-water-energy-cycle via formic acid intermediate by using the water-gas-shift reaction.



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Lecture at ICR
Breakthrough toward Chemical Connection of Aromatic Rings



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Lecture at ICR
Absolute Configuration of Organic Compounds: Elucidation Methods Evolved from Students' Studies



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Lecture at ICR
Structure and Dynamics of Polymer Gel



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Lecture at ICR
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ABC Transporter Structure & Function



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Lecture at ICR
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Quantum Hall Effect in Graphene



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Lecture at ICR
Computational Biophysics of Protein-Membrane Complex Systems



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Lecture at ICR
Local Structure Analysis of Wire-laminated Part in ULSI by STEM-EELS



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Associate Professor, Department of Global Epidemiology, Research Center for Zoonosis Control, Hokkaido University
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Lecture at ICR
Prediction of the Mutation of the Influenza Virus Gene



PERSONAL

Retirement

Professor ISODA, Seiji

Advanced Research Center for Beam Science

— Electron Microscopy and Crystal Chemistry —



On 31 March, 2010, Dr. Seiji Isoda retired from Kyoto University after 35 years of service and was honored with the title of Professor Emeritus of Kyoto University. Dr. Isoda was born in Kumamoto Prefecture on 5 January, 1947. He graduated from Department of Physics, Faculty of Science, Tohoku University in 1969 and subsequently entered the Graduate School of Science, Kyoto University, where he studied polymer physics under the supervision of late Professor Kenjiro Asai. In 1983, he was granted the doctoral degree for the thesis entitled “Epitaxial Synthesis of Poly(p-xylylene)”. In 1975, he was appointed Research Associate in the Institute for Chemical Research, Kyoto University, and he was promoted to Assistant Professor in 1983 and to Associate Professor in 1989. In 2001, he was appointed Professor in the Institute for Chemical Research, Kyoto University and directed the Laboratory of Electron Microscopy and Crystal Chemistry. Meanwhile, from 2005 to 2006, he served concurrently as the head of the Advanced Research Center for Beam Science.

Through his academic career, Dr. Isoda devoted himself to crystal chemistry using many types of microscope, focusing on structural analysis, growth mechanism and process of structural transformation of materials. Especially, he established the high resolution electron microscopy for organic materials by developing the image processing, the rapid correction of astigmatism of objective lens in high-voltage transmission electron microscope. Owing to the development of new methods, he realized the direct observation of organic molecules in thin film crystals at an 0.1 nm resolution, which opened the study of structural analysis at local area such as defects and interfaces in organic crystals based on the high resolution images.

He also contributed to further development in the electron crystallography based on the electron diffraction

using a special electron detector, which was applied to structure determination of perylene derivatives and many other organic thin films or fine particles. In order to improve the resistance of organic materials to electron irradiation, he developed a cryogenic transmission electron microscopy, observing the specimen at liquid helium temperature. He made pioneering work in local structure analyses of polymerization process and the low temperature phase of organic crystals. This cryogenic observation method was combined with the rapid cooling of samples, which made it possible to observe metal clusters in liquid and crystals including water.

He extended his study to surface structure at the initial stage of epitaxial growth by using scanning probe microscopy. He found a new epitaxial mode called point-on-line coincidence and clarified growth modes in terms of the lattice interaction on substrate and intermolecular interaction using computational science approach. With his deep knowledge on crystal growth mechanism, he further investigated organic field effect transistors and organic photoelectric conversion devices, focusing on the development of new device structure with high efficiency.

Throughout his career, Dr. Isoda’s scientific achievements were published in 206 original papers. He was frequently invited to international conferences and collaborated with many foreign scientists from England, Germany and China and so on. He also contributed to various scientific meetings and international congresses as an executive committee member. He served as a member of the editorial board of the journal published from the Japanese Society of Microscopy.

Dr. Isoda’s contribution to Kyoto University and the Institute through his scientific, educational and administrative activities is greatly acknowledged.

Awards

SASAMORI, Takahiro



Progress Award in Silicon Chemistry, Japan

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

The Society of Silicon Chemistry, Japan

31 October 2009

ONO, Teruo



The 27th Osaka Science Prize

“Pioneering Work on the Magnetization Control by Electric Currents”

Osaka Prefecture, Osaka City and Osaka Science & Technology Center

11 September 2009

YUASA, Akihiro



CSJ Student Presentation Award 2009

The 89th Annual Meeting of the Chemical Society of Japan

“Synthesis, Structure, and Properties of Stable 1,2-Bis-(metallocenyl)disilenes”

The Chemical Society of Japan

13 April 2009

KOBAYASHI, Kensuke



The 3rd Young Scientist Award of the Physical Society of Japan

“Experimental Study on the Controlling of the Coherence and the Many-body Effects of Electrons in Semiconducting Mesoscopic Systems”

Physical Society of Japan

28 March 2009

URUNO, Yoshiharu



Impressive Oral Presentation Award

The 39th Congress of Heterocyclic Chemistry

“Creation of a Peptide[2]catenane Based on Alternating D,L-Peptide Architecture”

The Organizing Committee of the 39th Congress of Heterocyclic Chemistry

16 October 2009

CHIBA, Daichi



The 4th Condensed-Matter Science Prize

“Experimental Study on the Electric Field Effect in Ferromagnetic Semiconductors”

Condensed-Matter Science Prize Office

29 November 2009

DELMO, Michael Picazo



ICR Award for Graduate Students

“Large Positive Magnetoresistive Effect in Silicon Induced by the Space-charge Effect”

Institute for Chemical Research, Kyoto University

4 December 2009

NISHIDA, Koji



The Award of the Society of Fiber Science and Technology, Japan

Annual Meeting, the society of Fiber Science and Technology, Japan

“In Situ Observation of Structure Formation in Fibers and Films”

The Society of Fiber Science and Technology, Japan

10 June 2009

YAMAZOE, Sayumi



ICR Award for Graduate Students

“A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth”

Institute for Chemical Research, Kyoto University

4 December 2009

MASUBUCHI, Yuichi



2009 Award of the Molecular Simulation Society of Japan

“Efficient Coarse-grained Simulations for Entangled Polymer Dynamics”

The Molecular Simulation Society of Japan

1 December 2009

NAKAGAWA, Yusuke



Sasakawa Scientific Research Encouragement Prize

“Stable Isotopic Marine Geochemistry of Molybdenum and Tungsten”

The Japan Science Society

30 April 2009

IKENOUCI, Junichi



Young Scientist Award for the Presentation

The 61st Annual Meeting of Japan Society for Cell Biology

“Determination of Lipid Compositions of Particular Membrane Domains in Epithelial Cells”

Japan Society for Cell Biology

3 June 2009

Paper Awards

IWASHITA, Yoshihisa



Nishikawa Prize

“Development of an Optical Inspection System for Superconducting RF Cavities and Surface Observation”

Foundation for High Energy Accelerator Science

23 March 2009

TOKITA, Shigeki



ICR Award for Young Scientists

“Single-Shot Ultrafast Electron Diffraction with a Laser-Accelerated Sub-MeV Electron Pulse”

Institute for Chemical Research, Kyoto University

4 December 2009

INOUE, Satoru



The Incentive Award for Excellent Presentation

The 69th Autumn Meeting of the Japan Society of Applied Physics

“Epitaxial Thin Film of SrFeO₂ with FeO₂ Infinite Layers by CaH₂ Low Temperature Reduction”

The Japan Society of Applied Physics

31 March 2009

YAMADA, Yasuhiro



ICR Award for Young Scientists

“Nonlinear Carrier Dynamics in Perovskite-oxide SrTiO₃”

Institute for Chemical Research, Kyoto University

4 December 2009

YUASA, Akihiro

SASAMORI, Takahiro

TOKITOH, Norihiro



BCSJ Award

“Synthesis and Properties of Stable 1,2-Bis(metallocenyl)disilenes: Novel d- π Conjugated Systems with a Si=Si Double Bond”

The Chemical Society of Japan

15 July 2009

KASAI, Shinya

NAKANO, Kunihiro

KONDOU, Kouta

OHSHIMA, Norikazu

KOBAYASHI, Kensuke

ONO, Teruo



MSJ Distinguished Paper Award

“Time-resolved Measurement of the Magnetic Vortex Core Dynamics by Using the TMR Effect”

Magnetic Society of Japan

13 September 2009

MATSUNAGA, Ryusuke



Incentive Award for Excellent Presentation

Oyo Butsuri Gakkai

“Observation of Dark Excitons in Single Carbon Nanotubes due to the Aharonov-Bohm Effect”

The Japan Society of Applied Physics

8 September 2009

Poster Awards

MIEDA, Eiko



The Best Poster Award

The 13th Symposium of the Society of Silicon Chemistry, Japan
“Studies on the Synthesis of 1,2-Diarylsilyne Bearing Bulky Substituents”

The Society of Silicon Chemistry, Japan

31 October 2009

MORINAKA, Yuta



The Best Poster Award

20th Symposium on Physical Organic Chemistry
“[4+2] Cycloaddition Reactions of Fullerene C₇₀ Encapsulating One and Two Molecules of Hydrogen”

Organization Committee of Physical Organic Chemistry

30 September 2009

URUNO, Yoshiharu



Impressive Poster Presentation Award

The 5th Host Guest Chemistry Symposium
“Toward the Development of Unique Materials Based on Alternating D,L-Peptide Architecture”

Association of Research for Host-Guest and Supramolecular Chemistry, Japan

30 May 2009

Best Poster Award

The 29th Seminar on Synthetic Organic Chemistry for Young Scientists

“The Creation of a Peptide[2]catenane and D,L-Peptide Catalysts Based on Alternating D,L-Peptide Architecture”

The Society of Synthetic Organic Chemistry, Japan

24 November 2009

AZUMA, Yusuke



The Best Poster Award

The 19th Symposium on Role of Metals in Biological Reactions, Biology and Medicine (SRM2009)
“Metal-Induced DNA-Binding Switch of bZIP Proteins Modified with Iminodiacetic Acid (Ida)”

The Pharmaceutical Society of Japan

12 June 2009

NAKAMURA, Atsushi



The Best Poster Award

The 16th Annual Meeting of Japanese Society for Chronobiology
“Creation of Artificial Zinc Finger-Type Transcription Factors towards Promoter Analysis of Clock Genes”

Japanese Society for Chronobiology

27 October 2009

YAMAZOE, Sayumi



Poster Prize

4th Annual Meeting of Japanese Society for Chemical Biology
“Discovery and Mechanism of Adhesamine, a Dumbbell-shaped Small Molecule that Promotes Cell Adhesion”

Japanese Society of Chemical Biology

19 May 2009

Poster Prize

The 25th Naito Conference
“A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth”

The Naito Foundation

11 September 2009

Incentive Award

51st Symposium of the Chemistry of Natural Products Nagoya 2009

“A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth”

The Chemistry of Natural Products

9 October 2009

SHINTANI, Megumi



Poster Prize

32nd Symposium on Solution Chemistry of Japan
“How Does the Molecular Binding into Model Membranes Depend on the Curvature?”

The Japan Association of Solution Chemistry

19 November 2009

KAWAMOTO, Jun



Poster Presentation Award

The 10th Annual Meeting of Japan Society of Extremophiles
“Physiological Role of Eicosapentaenoic Acid-containing Phospholipids in Refolding of a Cold-inducible Porin”

Japan Society of Extremophiles

28 October 2009

INOUE, Rintaro



The Best Poster Presentation Award

The 40th Summer School of the Society of Fiber Science and Technology, Japan

“Distribution of Glass Transition Temperature of Polymer Thin Film by Neutron Reflectivity”

The Society of Fiber Science and Technology, Japan

28 August 2009

ASAKAWA, Harutoshi



The Poster Presentation Award

The 40th Summer School of the Society of Fiber Science and Technology, Japan

“Crystallization Behavior from Mesomorphic Isotactic Polypropylene during Heating Process”

The Society of Fiber Science and Technology, Japan

28 August 2009

UNO, Akiko



The Best Presentation Award

The 2009 Annual Meeting of the Society of Rheology, Japan

“Estimation of Polystyrene Segment Size Detected by Dielectric Measurement”

The Society of Rheology, Japan

14 May 2009

HIRAMOTO, Keisuke



The Best Presentation Award in the 2009 Autumn Meeting of the Society of Rheology, Japan

“Dynamic Behavior of Polyisoprene and Poly(4-tert-butylstyrene) Blends; A study of Local Heterogeneity”

The Society of Rheology, Japan

6 October 2009

SOUDA, Hikaru



Poster Award

GCOE Opening Symposium

“Laser Cooling Experiment of $^{24}\text{Mg}^+$ Beam with Resonant Coupling”

Global COE Program “The Next Generation of Physics, Spun from Universality and Emergence”

18 February 2009

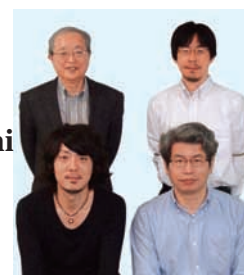
HARUTA, Mitsutaka

KURATA, Hiroki

KOMATSU, Hiroshi

SHIMAKAWA, Yuichi

ISODA, Seiji



Best Poster Award

EDGE2009: International EELS-Workshop

“Site Resolved Oxygen K-edge ELNES of Layered Double Perovskites $\text{La}_2\text{CuSnO}_6$ ”

International EELS-Workshop Committee

21 May 2009

POOLSAP, Unyanee

KATO, Yuki

AKUTSU, Tatsuya



Oxford Journals – JSBi Bioinformatics Prize (Best Poster Award)

The 20th International Conference on Genome Informatics

“Dynamic Programming Algorithms for RNA Structure Prediction with Binding Sites”

Japanese Society for Bioinformatics (JSBI)

16 December 2009

Obituary

Professor Emeritus

Dr. ODANI, Hisashi (1928–2009)



Dr. Hisashi Odani, Professor Emeritus of Kyoto University, passed away unexpectedly on August 27, 2009, in Kyoto.

Dr. Hisashi Odani was born in Kyoto on October 12, 1928. He graduated from Department of Industrial Chemistry, Kyoto University in 1952 and continued his studies on physicochemical properties of polymers as a graduate student at the same department under the supervision of Professor Mikio Tamura. After the graduation, he was appointed an instructor of the Faculty of Engineering, Kyoto University in 1957 and received a doctoral degree from Kyoto University for his studies on sorption of low-molecular-weight compounds in solid polymers including polymer membranes in 1962. He was promoted to Associate Professor in the same faculty in 1963 and moved to the Institute for Chemical Research, Kyoto University in 1966. He made a leave stay at the Institute of Physical Chemistry, Uppsala University in 1968 and worked for two years on fluorescence depolarization in sheared solutions of dye-tagged polymers in cooperation with Professor S. Claesson. In 1987, Dr. Odani was promoted to Full Professor of Kyoto University to direct the Laboratory of Fundamental Materials Properties, Institute for Chemical Research until his retirement. He retired from Kyoto University on March 31, 1992 and was honored with the title of Professor Emeritus of Kyoto University on the next day.

Dr. Odani conducted extensive researches in both fundamental and applied fields of polymer materials science, physical chemistry, and membrane science. In particular, he obtained prominent results in studying sorption and

de-sorption of low-molecular-weight compounds in solid polymers, visco-elasticity of solid polymers, solution properties of polymers, and diffusion, transport, and dissolution of gases, vapors, and their mixtures to polymer membranes, and contributed to important progresses in the research fields. Since these achievements were highly appreciated internationally as well as domestically, he was frequently invited to American Chemical Society Meetings, IUPAC Symposia, Polymer International Congresses and so on. Dr. Odani gave lectures on physical chemistry and fundamental materials science at the Faculty of Engineering, Kyoto University and on advanced materials science and polymer physics at the Graduate School of Engineering and he supervised dissertation works of many graduate students. He was also a visiting lecturer in Osaka University, Kyoto Institute of Technology, Ochanomizu Women's University, Yamaguchi University, and Nagasaki University.

Dr. Odani was an active member of the Chemical Society of Japan, the Society of Polymer Science, Japan, the Society of Rheology, Japan, the Society of Fiber Science and Technology, and so on. He served as a vice-president of the Society of Rheology, Japan, for two years since May, 1989 and also as a regular organizer of the Kinki Branch of the Chemical Society of Japan. He also contributed to *Journal of the Society of Rheology, Japan*, as an editor.

Dr. Odani was a gentle and sincere professor. His sincere and warm personality has won him the respect of his friends, colleagues, and students.

Obituary

Professor Emeritus

Dr. ODA, Jun'ichi (1934–2009)



Dr. Jun'ichi Oda, Professor Emeritus of Kyoto University, passed away on October 21, 2009, in Kyoto.

Dr. Jun'ichi Oda was born in Kyoto on December 20, 1934. After graduating from the Faculty of Agriculture, Kyoto University in 1959, he continued his studies on the synthesis and evaluation of biologically active natural products as a graduate student. In 1965, he was appointed Research Associate of the Laboratory of Plant Product Chemistry, Institute for Chemical Research, Kyoto University, under the supervision of late Emeritus Professor Minoru Ohno. Dr. Oda was conferred a doctoral degree from Kyoto University in 1965 for his studies on the synthesis of naturally occurring cumarane compounds. From 1968 to 1969 while he was on leave from Kyoto University, he stayed at the Department of Chemistry, Bonn University in West Germany and studied the metabolism of chlorinated hydrocarbon insecticides with Professor F. Korte. In 1973, Dr. Oda was promoted to Associate Professor of the same laboratory in Kyoto University. In 1984, he was appointed Professor of Kyoto University and directed the Laboratory of Plant Product Chemistry (present name, Chemistry of Molecular Biocatalysts), Institute for Chemical Research, Kyoto University. From April 1, 1992, to March 31, 1993, Dr. Oda was appointed Director of the Institute and made great contributions not only to the institute but also to the university as a councilor. He retired from Kyoto University and received Title of Professor Emeritus of Kyoto University in April 1998. After the retirement, he served as a professor and the dean of Graduate School of Bioscience and Biotechnology, Fukui Prefectural University from 1998 to 2005.

During the past 40 years, Dr. Oda's research interest encompassed a wide array of natural sciences including synthetic organic chemistry, stereochemistry, bioorganic chemistry, molecular biology, and structural biology. Following his early studies on the synthesis of biologically active plant products, he developed a series of asymmetric reactions such as Simmons-Smith reaction, cyclopropana-

tion, and a sigmatropic rearrangement. He synthesized a series of chiral dihydronicotinamide (NADH) derivatives as the model coenzyme of alcohol dehydrogenase, and carried out the stereoselective reduction of ketones with high enantioselectivity. He also focused on the use of lipases as a chiral catalyst in organic synthesis and prepared several important chiral synthons. As for the molecular biological aspect of his research, he cloned the gene of a microbial lipase and characterized a hitherto unknown protein which might assist the folding of the lipase specifically. He also prepared the catalytic antibodies which are capable of stereoselective hydrolysis of esters and carbonates, and defined the mechanisms of the catalyzed reaction and product inhibition. His research interest in enzyme chemistry and structural biology was highlighted by the X-ray crystallography of ATP-dependent ligases such as glutathione synthetase and asparagine synthetase. He also designed and synthesized transition-state analogue inhibitors of these ligases and used them for the elucidation of the detailed reaction mechanisms of the ligases by enzyme kinetics and structural characterization of the enzyme-inhibitor complex, along with time-resolved X-ray crystallography by Laue diffraction. All in all, he pioneered the interdisciplinary area of chemistry and biology; he has been engaged not only in green chemistry in which development of novel biocatalysts to archive environmentally friendly chemical synthesis but also in chemical and structural biology to unveil the nature of biologically important enzymes based on their atomic structures. For his brilliant achievements on biocatalysts, he was honored with the Senior Scientist Award from Japan Society for Bioscience, Biotechnology, and Agrochemistry in 1996.

Dr. Oda was a gentle and sincere man. He educated and mentored a lot of capable students and young scientists. The Japanese Government made public recognition of his achievements by the Order of the Sacred Treasure, "Zuihouchujushou" medal and granted the Senior Grade of the Fourth Court Rank in 2009.



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

THESSES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

- Tanabe T, Mizuhata Y, Takeda N, Tokitoh N: Syntheses and Structures of Overcrowded Silanedichalcogenols and their Applications to the Syntheses of Silanedichalcogenolato Complexes, *J. Organomet. Chem.*, **694**, 353-365 (2009).
- Mizuhata Y, Inamura K, Tokitoh N: Reaction of 9-Germaphenanthrene with Dimethyl Acetylenedicarboxylate: Unexpected Formation of a 1,2-Oxagermolane Derivative, *Heterocycles*, **77**, 811-816 (2009).
- Tokitoh N, Tsurusaki A, Sasamori T: A Unique Thermal Reaction of 9-Anthryldiphosphene Leading to the Formation of a Triphosphirane Derivative, *Phosphorus Sulfur and Silicon and the Related Elements*, **184**, 979-986 (2009).
- Tokitoh N, Kawai M, Takeda N, Sasamori T: Intramolecular Si-C and C-H Bond Activation in a Platinum Complex Leading to the Formation of the Platinacycles, *Heterocycles*, **79**, 311-318 (2009).
- Tsurusaki A, Sasamori T, Tokitoh N: [4+2] Cycloaddition of 9-Anthryldiphosphene with Electron-Deficient Olefins: Transformation of a Diaryldiphosphene to Alkylaryldiphosphenes, *Organometallics*, **28**, 2604-3607 (2009).
- Yuasa A, Sasamori T, Hosoi Y, Furukawa Y, Tokitoh N: Synthesis and Properties of Stable 1,2-Bis(metalloacenyl)disilenes: Novel $d-\pi$ Conjugated Systems with a Si=Si Double Bond, *Bull. Chem. Soc. Jpn.*, **82**, 793-805 (2009).
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- Mizuhata Y, Shinohara A, Tanabe Y, Tokitoh N: Cycloaddition Reactions of Kinetically Stabilized 9-Silaanthracene with Polycyclic Aromatic Hydrocarbons, *Chem. Eur. J.*, **15**, 8405-8408 (2009).
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- Hayashi S, Nakanishi W, Furuta A, Drabowicz J, Sasamori T, Tokitoh N: How Does Non-covalent Se...Se=O Interaction Stabilize Selenoxides at Naphthalene 1,8-positions: Structural and Theoretical Investigations, *New J. Chem.*, **33**, 196-206 (2009).
- Tsutsumi J, Sasamori T, Yoshida H, Tokitoh N, Sato N, Kato S, Muzikante I, Neilands O: A Noncentrosymmetric Crystal Structure of a Zwitterionic Compound, Pyridinium 5,7-dihydro-5,7-dioxo-6H-cyclopenta[b]pyridin-6-ylide, Realized by Weak Hydrogen Bonds, *J. Mol. Struct.*, **920**, 52-60 (2009).
- Hiroto S, Aratani N, Shibata N, Higuchi Y, Sasamori T, Tokitoh N, Shinokubo H, Osuka A: Zwitterionic Corroles: Regioselective Nucleophilic Pyridination of a Doubly Linked Biscorrole, *Angew. Chem. Int. Ed.*, **48**, 2388-2390 (2009).
- Hiramatsu T, Sasamori T, Yoshida H, Tokitoh N, Sato N: Reversible Polymorphic Crystalline Transition of a Push-pull-type Molecule: {4-[4,5-bis(methylsulfanyl)-1,3-dithiol-2-ylidene]Cyclohexa-2,5-dien-1-ylidene}Malononitrile (BMDCM), *J. Mol. Struct.*, **922**, 30-34 (2009).
- Nakazono S, Imazaki Y, Yoo H, Yang J, Sasamori T, Tokitoh N, Cedric T, Kageyama H, Kim D, Shinokubo H, Osuka A: Regioselective Ru-Catalyzed Direct 2,5,8,11-Alkylation of Perylene Bisimides, *Chem. Eur. J.*, **15**, 7530-7533 (2009).
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- Maeda C, Kamada T, Aratani N, Sasamori T, Tokitoh N, Osuka A: Selective Formation of a Single Atropisomer of *meso-meso*-Linked Zn(II) Diporphyrin through Supramolecular Self-Assembly, *Chem. Eur. J.*, **15**, 9681-9684 (2009).

— Structural Organic Chemistry —

Margetic D, Murata Y, Komatsu K, Marinic Z: Rigid Alicyclic Molecules from Bicyclo[2.2.1]hept-2-enes (=8,9,10-Trinorbornenes) and 1,4-Dipyridin-2-ylphthalazines as Stereoselective Coupling Agents, *Helv. Chim. Acta*, **92**, 298-312 (2009).

Horsewill AJ, Panesar KS, Rols S, Johnson MR, Murata Y, Komatsu K, Mamone S, Danquigny A, Cuda F, Maltsev S, Gressel MC, Carravetta M, Levitt MH: Quantum Translator-Rotator: Inelastic Neutron Scattering of Dihydrogen Molecules Trapped inside Anisotropic Fullerene Cages, *Phys. Rev. Lett.*, **102**, [013001-1]- [013001-4] (2009).

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— Synthetic Organic Chemistry —

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

- Sue D, Takaishi K, Harada T, Kuroda R, Kawabata T, Tsubaki K: Synthesis of Chiral Dotriacontanaphthalenes: How Many Naphthalene Units are We Able to Elaborately Connect?, *J. Org. Chem.*, **74**, 3940-3943 (2009).
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- [Others]
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- DIVISION OF MATERIALS CHEMISTRY**
— Chemistry of Polymer Materials —
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Department of Electrical and Computer Engineering, National University of Singapore

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[Spain]
CIC nano GUNE Consolider, San Sebastian

Institut de Recerca Biomèdica, Parc Científic de Barcelona

[Sweden]
Department of Neurochemistry, Stockholm University

[Switzerland]
Solid State Physics Laboratory, ETH Zürich

[Thailand]
Faculty of Science, Mahidol University

Faculty of Science, Prince of Songkla University

[U.K.]
Centre for Science at Extreme Conditions, The University of Edinburgh

Department of Physics and Astronomy, University of Leeds

Institute for Complex Systems and Mathematical Biology, University of Aberdeen

ISIS Facility, Rutherford Appleton Laboratory

School of Chemistry, Southampton University

University of Oxford

Welsh School of Pharmacy, Cardiff University

[U.S.A.]
Biochemistry and Molecular Biology, Baylor College of Medicine

Department of Chemistry, Brown University

Department of Chemistry, Columbia University

Department of Chemistry, University of Florida

Department of Chemistry and Bioengineering, Rice University

Department of Materials, University of California

LANSCE, Los Alamos National Laboratories

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

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

THESES

- HASHISAKA, Masayuki
D Sc, Kyoto University
“Precise Measurement of Quantum Shot Noise in Mesoscopic Systems”
Supervisor: Assoc Prof KOBAYASHI, Kensuke
23 March 2009
- HIRAKAWA, Mika
D Sc, Kyoto University
“Development of Informatics Resources for Human Genome Research and Analysis of Retroposons Conserved in Noncoding Regions of the Mammalian Genome”
Supervisor: Prof KANEHISA, Minoru
25 May 2009
- HIRAMATSU, Takaaki
D Sc, Kyoto University
“A Study on Molecular Properties and Aggregation Behaviors of an Amphoteric Polar Molecule, BMDCM”
Supervisor: Prof SATO, Naoki
25 May 2009
- KAN, Keizo
D Pharm Sc, Kyoto University
“Development of Chiral Nucleophilic Catalysts with Functionalized Side Chains for Substrate Recognition”
Supervisor: Prof KAWABATA, Takeo
23 March 2009
- KAWAI, Masahiro
D Sc, Kyoto University
“Synthesis and Application of Transition Metal Complexes Bearing Overcrowded Phosphine Ligands”
Supervisor: Prof TOKITOH, Norohiro
23 March 2009
- MOURI, Kazunari
D Inf, Kyoto University
“Analyses of the Effects of Fluctuation in Biological Systems”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2009
- OMORI, Taketo
D Agr, Kyoto University
“Biochemical Studies of Novel Glycerophospholipids in Mammals”
Supervisor: Assoc Prof KURIHARA, Tatsuo
23 July 2009
- OZAKI, Shuhei
D Sc, Kyoto University
“Studies on the Synthesis and Properties of Kinetically Stabilized 1-Hydrosilene”
Supervisor: Prof TOKITOH, Norohiro
23 March 2009
- RAHMAN, Nelly
D Eng, Kyoto University
“Studies on Crystallization of Poly(Lactic Acid) and Related Polymers”
Supervisor: Prof KANAYA, Toshiji
23 March 2009
- SHIGEMIZU, Daichi
D Sc, Kyoto University
“Extraction and Analysis of Chemical Modification Patterns in Drug Development”
Supervisor: Prof KANEHISA, Minoru
24 November 2009
- TAKAHASHI, Hideaki
D Eng, Kyoto University
“Linear and Nonlinear Rheological Properties of Scarcely Crosslinked Poly (dimethyl siloxane) Gels”
Supervisor: Prof WATANABE, Hiroshi
23 March 2009
- TANABE, Taro
D Sc, Kyoto University
“Syntheses of Silanedichalcogenolato Transition Metal Complexes Utilizing Stable Silanedichalcogenols and Elucidation of Their Structures and Reactivities”
Supervisor: Prof TOKITOH, Norohiro
23 March 2009
- TANIGAWA, Hironobu
D Sc, Kyoto University
“Current-induced and Magnetic-field-induced Magnetic Domain Wall Motion in Ferromagnetic Nano-Wire with Perpendicular Magnetic Anisotropy or In-plane Magnetization”
Supervisor: Prof ONO, Teruo
23 March 2009
- TOBE, Ryuta
D Agr, Kyoto University
“Enzymological Studies on Selenoprotein Biosynthesis”
Supervisor: Assoc Prof KURIHARA, Tatsuo
23 July 2009
- TSUTSUMI, Jun'ya
D Sc, Kyoto University
“Solid-State Structures and Electronic Properties of Organic Molecules Fabricated by Connecting Electron Donor and Acceptor Components”
Supervisor: Prof SATO, Naoki
23 January 2009
- WAKIOKA, Masayuki
D Eng, Kyoto University
“Synthesis and Photochemical Properties of Poly(phenylenevinylene)s with Highly Regulated Structures”
Supervisor: Prof OZAWA, Fumiyuki
24 September 2009
- WATANABE, Toshihide
D Pharm Sc, Kyoto University
“Asymmetric Synthesis of Amino Acid Derivatives with Tetra-substituted Carbon via Memory of Chirality”
Supervisor: Prof KAWABATA, Takeo
23 March 2009

YAMAUCHI, Takae
D Agr, Kyoto University
“Structure and Function of Serine Racemase”
Supervisor: Assoc Prof KURIHARA, Tatsuo
23 July 2009

YUASA, Akihiro
D Sc, Kyoto University
“Construction of New Redox Systems Utilizing the Properties of
Low-coordinated Heavier Group 14 Compounds”
Supervisor: Prof TOKITOH, Norohiro
23 March 2009



THE 109TH
ICR ANNUAL
SYMPOSIUM

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MEETINGS AND
SYMPOSIA



THE 109TH ICR ANNUAL SYMPOSIUM

(4 December 2009)

ORAL PRESENTATIONS

HIRAI, Asako (Molecular Materials Chemistry)
“Control of Crystal Polymorphs of Bacterial Cellulose and Their Resultant Higher Order Structures”

INOUE, Rintaro (Polymer Materials Science)
“Glass Transition of Polymer Thin Film”

TOKUDA, Youmei (Inorganic Photonics Materials)
“Structure Engineering and Material Function Controlling of Organic-inorganic Hybrid Materials”

SOUDA, Hikaru (Particle Beam Science)
“Transverse Laser Cooling of $^{24}\text{Mg}^+$ Beam by Resonant Coupling”

TAKIGAWA, Ichigaku (Pathway Engineering)
“Metabolic Pathway Estimation Using Gene Expression”

M. Lutfi Firdaus, et al. (Trace Elemental Tomography)
“Sectional Distribution of Zr, Hf, Nb, Ta, Mo and W in the Southern and South Pacific Ocean”

KURIHARA, Tatsuo (Molecular Microbial Science)
“How Microbes Survive in the Antarctic?”




– ICR Award for Young Scientists –
TOKITA, Shigeki (Laser Matter Interaction Science)
“Single-shot Ultrafast Electron Diffraction with a Laser-accelerated Sub-MeV Electron Pulse”

YAMADA, Yasuhiro (Photonic Elements Science)
“Temperature Dependence of Photoluminescence Spectra of Nondoped and Electron-Doped SrTiO_3 : Crossover from Auger Recombination to Single-Carrier Trapping”


– ICR Award for Graduate Students –
DELMO, Michael Picazo (Nanospintronics)
“Large Positive Magnetoresistive Effect in Silicon Induced by the Space-charge Effect”


YAMAZOE, Sayumi (Chemical Biology)
“A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth”

POSTER PRESENTATIONS


 : Laboratory Whole Presentation
 : Laboratory Topic
 : General Presentation


— Organoelement Chemistry —

 “Synthesis and Properties of Novel Organic Compounds Containing Heavy Elements”


 MIEDA, Eiko; SASAMORI, Takahiro; TOKITOH, Norihiro
“Studies on the Synthesis of 1,2-Diarylsilyne Bearing Bulky Substituents”


— Structural Organic Chemistry —

 MORINAKA, Yuta; MURATA, Michihisa; KUROTOBI, Kei; MURATA, Yasujiro
“Chemical Transformation of Cage-Opened Fullerene by Grignard Reagents”


 KUROTOBI, Kei; YASUI, Hidefumi; MURATA, Yasujiro
“Design and Synthesis of New Fullerene Derivatives with Extended π -System”


— Synthetic Organic Chemistry —

 YAMAMOTO, Junya; KITAMURA, Yuki; HASHIMOTO, Ayano; FURUTA, Takumi; MASU, Hyuma; AZUMAYA, Isao; KAN, Toshiyuki; KAWABATA, Takeo
“Efficient Synthesis of Axially Chiral Amino Acid and Alcohol through Pd-catalyzed Domino Coupling Reaction”


 SUE, Daisuke; KAWABATA, Takeo; TSUBAKI, Kazunori
“Synthesis of the Spirolactone Compounds via a Novel Framework Rearrangement Reaction”

— Chemistry of Polymer Materials —

 SHINJO, Ayaka; NAGASAWA, Kouji; GOTO, Atsushi; TSUJII, Yoshinobu; FUKUDA, Takeshi
“Living Radical Polymerization with Carbon Catalysts–Reversible Chain Transfer Catalyzed Polymerization”

 KIM, Jeongsik; GOTO, Atsushi; HIRAI, Asako; TSUJII, Yoshinobu; FUKUDA, Takeshi
“Surface-initiated Living Radical Polymerization from Cellulose Nanofiber”

— Polymer Controlled Synthesis —

 WATANABE, Yoshiki; IWAMOTO, Takahiro; YAMAGO, Shigeru
“Synthesis of Cycloparaphenylenes from Bis-Aryl Platinum Macrocyclic Complexes”

GE YAMADA, Hiroto; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Development and Application of Selective Transmetallation
of Heavier Heteroatom Compounds”

GE UEKI, Kazuya; YAMAGO, Shigeru
“Synthesis of Oligo(Aromatic Ketone)s by Iterative Friedel-
Crafts Reaction”

— Inorganic Photonics Materials —

LT SHINAGAWA, Masashi; TOKUDA, Youmei; TAKAHASHI,
Masahide; YOKO, Toshinobu
“Recent Research Topics in YOKO Laboratory”

— Nanospintronics —

GE CHIDA, Kensaku; HASHISAKA, Masayuki; YAMAUCHI,
Yoshiaki; NAKAMURA, Shuji; MACHIDA, Tomoki;
KOBAYASHI, Kensuke; ONO, Teruo
“Non-equilibrium Noise in the Regime of the Quantum Hall
Effect Breakdown”

GE YAMADA, Gen; KOYAMA, Tomohiro; UEDA, Kouhei;
TANIGAWA, Hironobu; FUKAMI, Shunsuke; SUZUKI,
Tetsuhiro; OHSHIMA, Norikazu; ISHIWATA, Nobuyuki;
CHIBA, Daichi; NAKATANI, Yoshinobu; KOBAYASHI,
Kensuke; ONO, Teruo
“Current-induced Motion of Multi Domain Walls in a Co/Ni
Wire with Perpendicular Magnetic Anisotropy”

GE TANABE, Kenji; CHIBA, Daichi; KASAI, Shinya;
KOBAYASHI, Kensuke; ONO, Teruo
“Detection of Spin Motive Force Induced by Magnetic
Vortex Dynamics”

— Biofunctional Design-Chemistry —

LW “Research Activity at Biofunctional Design Chemistry”

GE YU, Hao-Hsin; NAKASE, Ikuhiko; SILVIA, Pujals; IMANISHI,
Miki; FUTAKI, Shiroh
“Application of Expressed Protein Ligation to the Preparation
of Fusion Proteins with Arginine-rich Cell Penetrating
Peptides”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities in Chemistry of Molecular Biocatalysts”

— Molecular Biology —

LW “Recent Activities of Laboratory of Molecular Biology”

— Chemical Biology —

LW “Chemicalbiology”

GE SATO, Shinichi; MURATA, Asako; ORIHARA, Tsubasa;
SUENAGA, Kiyotake; KIGOSHI, Hideo; UESUGI, Motonari
“Isolating and Identifying Protein Targets of Marine Natural
Product Aurilide”

— Molecular Materials Chemistry —

LT SUZUKI, Furitsu; YAMADA, Tomonori; SATO, Tohru;
TANAKA, Kazuyoshi; KAJI, Hironori
“Charge Transfer Integrals and Charge Transport Paths in
Bipolar-transport and Hole-transport Materials for Organic
Light-emitting Diodes”

GE TAKAMI, Kosuke; KUSAKA, Yasunari; KUGA, Takako; KAJI,
Hironori
“Two-Dimensional Double-Quantum ¹⁵N Solid-State NMR
Characterization of Tris(8-hydroxyquinoline) Aluminum(III)
(Alq₃)”

GE KAWAGUCHI, Hisafumi; YAMADA, Tomonori; KAJI, Hironori
“Analysis of Mobility and Transport Process in an Organic
Charge Transport Material by Monte Carlo Calculation”

— Hydrospheric Environment Analytical Chemistry —

LT UMETANI, Shigeo; WATANABE, Kazuya; SOHRIN, Yoshiki
“Ion Imprinted Organic-inorganic Hybrid Adsorbent for the
Separation of Metal Ions”

— Solution and Interface Chemistry —

LT YASAKA, Yoshiro; WAKAI Chihiro; NAKAHARA, Masaru;
MATUBAYASHI, Nobuyuki
“Computational Study on the Slow Dynamics in Ionic Liquids”

GE KARINO, Yasuhito
“Free-energy Analysis of Solvent Effect on Structural Stability
of Protein”

— Molecular Microbial Science —

LT HIDESE, Ryota; MIHARA, Hisaaki; KURIHARA, Tatsuo;
ESAKI, Nobuyoshi
“Genome-wide Screening of the Essential Genes for Dihy-
dropyrimidine Dehydrogenase Activity”

LT SATO, Sho; KURIHARA, Tatsuo; OKAZAKI, Masaaki;
KAWAMOTO, Jun; OZAWA, Fumiyuki; ESAKI, Nobuyoshi
“Synthesis and Evaluation of Molecular Probe for Analyzing
the Function of Phospholipids Containing Eicosapentaenoic
Acid”

— Polymer Materials Science —

LW “Reserach Topics of Polymer Material Science Laboratory”

GE ZHAO, Yunfeng; MATSUBA, Go; NISHIDA, Koji; KANAYA,
Toshiji
“Study of Meso Structures in Isotactic Polystyrene Induced
by Shear Flow”

GE MORITA, Hideyuki; TANAKA, Kentaro; NISHIDA, Koji;
MATSUBA, Go; KANAYA, Toshiji
“Gelation and Phase Separation Behavior of Methylcellulose
Aqueous Solution with Added Salt”

— **Molecular Rheology** —

- GE KATAKURA, Shiro; CHEN, Quan; MATSUMIYA, Yumi; WATANABE, Hiroshi
“Dynamics of Disorderd PtBS-PI-PtBS Triblock Copolymer”
- GE HIRAMOTO, Keisuke; CHEN, Quan; MATSUMIYA, Yumi; WATANABE, Hiroshi
“Dynamics of Disorderd Polyisoprene/Poly(4-tert-butylstyrene) Blend”
- GE CHEN, Quan; MATSUMIYA, Yumi; WATANABE, Hiroshi
“Dynamics of Disorderd Diblock Copolymer: Poly(isoprene-b-4-tert-butyl styrene)”

— **Molecular Aggregation Analysis** —

- LT KAWAUCHI, Tatsuro; TSUTSUMI, Jun'ya; YOSHIDA, Hiroyuki; SATO, Naoki
“Crystal Structure of Dimethylamino-substituted Pyridinium 1,3-dihydro-1,3-dioxo-2H-inden-2-ylide (PI)”
- GE ASAMI, Koji
“Dielectric Spectroscopy of Biological Cells and Tissues”

— **Supramolecular Biology** —

- LW “Review of Current Research at Laboratory of Supramolecular Biology”
- GE YAMAMOTO, Masatoshi; KATO, Utako; UMEDA, Masato
“Phospholipid Flip-flop in Organelles and its Cellular Functions”

— **Particle Beam Science** —

- LW “Outline of Particle Beam Science Research Laboratory”
- GE YAMADA, Masako
“VCN-focusing-SANS with Modulating Magnetic Lens for Pulsed White Neutron Beams”

— **Laser Matter Interaction Science** —

- LW “Advances in Laser Matter Interaction Science”
- GE MIYASAKA, Yasuhiro; HASHIDA, Masaki; OKAMURO, Kiminori; TOKITA, Shigeki; SAKABE, Shuji
“Mechanism of Femtosecond Laser Nano Ablation for Metals ~Dependence of Ion Emission on Laser Polarization~”
- GE JAHANGIRI, Fazel; NAGASHIMA, Takeshi; HASHIDA, Masaki; TOKITA, Shigeki; HANGYO, Masanori; SAKABE, Shuji
“THz Radiation from Argon Clusters Irradiated by Intense Femtosecond Laser Pulses”
- GE OKAMURO, Kiminori; HASHIDA, Masaki; MIYASAKA, Yasuhiro; TOKITA, Shigeki; SAKABE, Shuji
“The Investigation of Mechanism of Periodic Nanostructure on Metal after Femtosecond Pulse Laser Irradiation”

- GE HIROKANE, Mayu; TOKITA, Shigeki; HASHIDA, Masaki; SAKABE, Shuji
“Development of High Power 3 μ m OH Absorption Band Tunable Fiber Laser”
- GE NISHOJI, Toshihiko; TOKITA, Shigeki; TAGUCHI, Toshihiro; INOUE, Shunsuke; OTANI, Kazuto; HASHIDA, Masaki; SAKABE, Shuji
“Measurement of the Angular Distributions of 100-keV-1-MeV Electron Emission from Intense Shortpulse Laserproduced Plasmas”
- GE INOUE, Shunsuke; TOKITA, Shigeki; NISHOJI, Toshihiko; MASUNO, Shinichiro; OTANI, Kazuto; HASHIDA, Masaki; SAKABE, Shuji
“Measurement of Spacial Distributions of Electron Sources in the Laser-plasma Interacted Region”

— **Electron Microscopy and Crystal Chemistry** —

- LW “Recent Research Topics of Division of Electron Microscopy and Crystal Chemistry”
- GE SHINODA, Yasuhiro; KURATA, Hiroki; SHIRAKI, Hiroshi; SHIMAKAWA, Yuichi; ISODA, Seiji
“EELS Study of CaCu₃B₄O₁₂ (B=Ti, Ge, Sn)”

— **Structural Molecular Biology** —

- LT HATA, Yasuo; KOBAYASHI, Kazutaka; YAMAUCHI, Takae; FUJII, Tomomi
“Structural Basis of Enzymes Involved in Catabolic Pathway of Resorcynol”

— **Organic Main Group Chemistry** —

- LW “Current Research Activities in Organic Main Group Chemistry Laboratory”
- GE HASHIMOTO, Toru; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
“Iron-Catalyzed Suzuki-Miyaura Coupling Reaction”
- GE SEIKE, Hirofumi; ISHIZUKA, Kentaro; ONITSUKA, Satoaki; HATAKEYAMA, Takuji; INANAGA, Junji; NAKAMURA, Masaharu
“Nickel-Catalyzed Alkenylative Cross-Coupling Reaction of Alkyl Sulfides”
- GE HASHIMOTO, Sigma; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
“Synthesis of Novel Hetero- π -conjugated Molecular Bowls”
- GE SASANO, Daisuke; SEIKE, Hirofumi; FUKUI, Sadayuki; OGATA, Kazuki; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Transition-Metal-Bound Peptide: Synthesis, Structure, and Function”

— **Advanced Solid State Chemistry** —

- LW “Activity of Solid State Chemistry Group”

- GE NAKAMURA, Yoshitaka; KAWAI, Masanori; AZUMA, Masaki; SHIMAKAWA, Yuichi
“Preparation and Characterization of (1-x)BiFeO₃-xBiCoO₃ Prepared by Chemical Solution Deposition”

— **Organotransition Metal Chemistry** —

- LW “Activity Report: Organotransition Metal Chemistry Laboratory”

- GE WAKIOKA, Masayuki; NAKAJIMA, Yumiko; OZAWA, Fumiyuki
“Mechanism of P-C Reductive Elimination from Styrylpalladium (II) Phosphine Complexes”

— **Photonic Elements Science** —

- LW “Research Topics in Photonic Elements Science”

— **Bioknowledge Systems** —

- LW “KEGG Database and GenomeNet Pharmaceutical Products Database”

— **Biological Information Networks** —

- GE POOLSAP, Unyanee
“Dynamic Programming Algorithms for RNA Structure Prediction with Binding Sites”

— **Pathway Engineering** —

- LT KAYANO, Mitsunori
“Genome-wide Three-way Gene Interactions from Transcript and Genotype Data”

— **Research Center for Low Temperature and Materials Sciences** —

- LT TERASHIMA, Takahito; KASAHARA, Shigeru; SHISHIDO, Hiroaki; YAMASHITA, Minoru; SHIBAUCHI, Takasada; MATSUDA, Yuji
“Preparation and Properties of Iron-pnictides Superconductors”

SEMINARS

Dr ABE, Fumiyoshi
Japan Agency for Marine-Earth Science and Technology, Yokosuka,
Japan
“Analysis of Biological Membrane Dynamics by Using High
Pressure and Fluorescence Depolarization Techniques”
20 October 2009

Prof ACKERMANN, Lutz
Institute of Organic and Biomolecular Chemistry, Georg-
August-Universität Göttingen, Göttingen, Germany
“Transition Metal-Catalyzed Direct Arylations via C-H Bond
Cleavages”
28 September 2009

Dr AOKI, Kazuhiro
Graduate School of Medicine, Kyoto University, Kyoto, Japan
“Quantitative Modeling of Cellular Signal Transduction”
21 May 2009

Assoc Prof ARITA, Makoto
Graduate School of Pharmaceutical Sciences, The University of
Tokyo, Tokyo, Japan
“Metabolomics of Pro-resolution Lipid Mediators”
26 October 2009

Prof ARNASON, Ingvar
University of Iceland, Iceland
“Organosilicon Chemistry in Iceland: Conformations and Complexes”
18 May 2009

Dr AUDIER, Marc
Grenoble Institute of Technology, France,
“Towards a Direct Fabrication of 3D Photonic Crystals!”
13 October 2009

Dr BOWIE, Andrew R
Antarctic Climate & Ecosystems CRC, University of Tasmania,
Australia
“Different Processes Drive Biogeochemical Iron Budgets in the
Subantarctic and Polar Southern Ocean during Summer”
30 March 2009

Prof CHAIRUANGSRI, Torranin
Department of Industrial Chemistry, Faculty of Science, Chiang
Mai University, Chiang Mai, Thailand
“Microstructural Study of Cast Metals in Thailand Using Electron
Microscopy: Current Status and Future Opportunity”
22 May 2009

Prof CHEN, Chun-Wei
Department of Materials Science and Engineering, National
Taiwan University, Taipei, Taiwan
“Nanostructured Metal Oxide/Polymer Hybrid Solar Cells”
10 July 2009

Prof CHEN, Jie-Sheng
School of Chemistry & Chemical Engineering, Shanghai Jiao
Tong University, Taiwan
“Pores Make Difference—Physical-Chemical Interactions inside
the Pores of Microporous and Mesoporous Materials”
15 September 2009

Prof CHEVELKO, Viatcheslav P
P. N. Lebedev Physical Institute of Russian Academy of Sciences,
Russia
“Multiple-electron Loss of Fast Heavy Ions in Collisions with
Neutral Atoms”
9 March 2009

Dr CHOU, Weiren
Fermi National Accelerator Laboratory, USA
“Accelerator Related Activities at Fermilab”
9 July 2009

Prof ERKER, Gerhard
Westfälische Wilhelms-Universität, Germany
“Frustrated Lewis-Pairs: Metal-free Activation of Dihydrogen
and More”
18 September 2009

Prof FERRÉ, Jacques
Laboratoire de Physique des Solides, Université Paris-Sud, Orsay,
France
“Domain Wall Motion in 2D Disordered Media: Creep, Depinning
and Flow Regimes”
11 June 2009

Prof GASTEIGER, Johann
University of Erlangen-Nuremberg, Germany
“Multidimensional Explorations into Biochemical Pathways”
30 November, 2009

Prof GATES, Derek P
University of British Columbia, Canada
“Low-coordinated Phosphorus Chemistry: From Molecules to
Polymers to Controlled Nanoassemblies”
31 August 2009

Prof GENZER, Jan
Department of Chemical & Biology Engineering, North Carolina
State University, USA
“Formation and Application of Multivariant Polymer Brush
Assemblies”
1 June 2009

Dr HASHIZUME, Daisuke
Riken, Japan
“Chemistry Powered by X-Ray Crystal Structure Analysis”
19 June 2009

Prof HUYNH, Vinh H
Department of Chemistry, National University of Singapore
(NUS), Singapore
“Determination of Donor Strengths on a Unified ¹³C NMR Scale
with NHC Complexes and Pyrazole-Based Remote Carbenes as
New Organometallic Ligands”
22 October 2009

Prof ITO, Shinzaburo
Department of Polymer Chemistry, Kyoto University, Kyoto, Japan
“Shapes and Distributions of Polymer Chains at Interfaces”
27 March 2009

- Prof IVANOV, Boris A.
Institute of Magnetism, Nat. Acad. Sci. of Ukraine, and Kiev State University, Ukraine
“High Frequency Magnon Modes for the Vortices in Ferromagnetic and Antiferromagnetic Particles: Structure and Excitation by Pulses of Magnetic Field and Spin-polarized Current”
28 October 2009
- Prof JONES, William D
University of Rochester, USA
“Strong C–H and C–C Bond Cleavage Using Homogeneous Transition Metal Complexes”
25 August 2009
- Prof JUNG, Myung-Hwa
Department of Physics, Sogang University, Seoul, Korea
“Proposal for a New Class of Spin Hall Material”
2 February 2009
- Prof KOST, Daniel
Ben-Gurion University of the Negev, Israel
“Penta- and Hexacoordinate Organosilicon Compounds: a Remarkably Flexible Molecular System”
15 October 2009
- Prof KRAUSE, Norbert
Dortmund University, Germany
“The Power of Gold”
11 November 2009
- Dr KUSMARTSEVA, Anna
Centre for Science at Extreme Conditions, University of Edinburgh
“High Pressure Synthesis and Properties of PbRuO₃”
11 September 2009
- Dr LEMIEGRE, Loic
Ecole Nationale Supérieure de Chimie de Rennes, France
“Archaeal Lipid Analogues: From Synthesis to Gene Delivery”
13 April 2009
- Dr LIU, Zhiping
Chinese Academy of Sciences, Beijing, China
Osaka Sangyo University, Osaka, Japan
“Dynamically Dysfunctional Protein Interactions in the Development of Alzheimer’s Disease”
16 July 2009
- Prof LODGE, Tim
Department of Chemistry and Department of Chemical Engineering & Materials Science
University of Minnesota, Minneapolis, USA
“Block Copolymer Micelles: Equilibrium and Non-equilibrium Assembly”
16 January 2009
- Ms LOMBARDI, Benedetta
University of Rome La Sapienza, Rome, Italy
“Regulation by the COP9 Signalosome of PIC2, a F-box Protein from *Arabidopsis thaliana*”
10 June 2009
- Prof MACHIDA, Tomoki
Institute of Industrial Science, The University of Tokyo, Japan
“Quantum Hall Effect in Graphene”
2 March 2009
- Dr MELE, Giovanni
IBBA Institute, National Research Council of Italy, Rome, Italy
“Does Brevipedicellus, Homeobox Gene, Define Intra-bundle Phloem and Xylem Localization”
6 April 2009
- Dr MELKMAN, Avraham
Computer Science Department, Ben Gurion University, Israel
“Integrating Gene Annotations into Data Analysis”
16 November 2009
- Prof MIYAURA, Norio
Graduate School of Engineering, Hokkaido University, Hokkaido, Japan
“Catalytic Chemistry of Organoboronic Acid”
28 September 2009
- Prof MORRIS, Robert H
Department of Chemistry, University of Toronto, Toronto, Canada
“Moving from Ruthenium Catalysts to Iron Catalysts for the Asymmetric Reduction of Ketones”
20 January 2009
- Assist Prof NAKAGAWA, Masato
Center for iPS Cell Research and Application, iCeMS, Kyoto University, Kyoto, Japan
“iPS Cell Research for Clinical Application”
23 July 2009
- Dr NAKAYA, Akihiro
The University of Tokyo, Japan
“KEGG OC: Automatic Generation of Comprehensive Ortholog Cluster”
27 April 2009
- Dr NG, See-Kiong
Institute for Incomm Research, A*STAR, Singapore
“Unraveling the Building Blocks of Protein-protein Interaction Networks”
20 April 2009
- Dr NICOLOPOULOS, Stavros
NanoMEGAS, Brussels, Belgium
“Precession Electron Diffraction–Phase and Orientation Mapping (“EBSD” Like TEM Technique)”
10 September 2009
- Dr OHIRA, Shino
School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA
“Theoretical Evaluation of the Nonlinear Optical Properties of Extended π -conjugated Chromophores”
29 October 2009
- Prof POEPPELMEIER, Kenneth
Northwestern University, USA
“Hydro/solvothermal Chemistry: Targeting Noncentrosymmetric Structures and Other New Materials”
26 May 2009
- Prof RHIE, Kungwon
Display and Semiconductor Physics, Korea University, Chochiwon, Korea
“Landau Level Induced Magnetoswitching Effect in High Mobility Semiconductor System”
2 February 2009

Prof RICHTER, Dieter
Institut für Festkörperforschung, Forschungszentrum Jülich, Germany
“Biomolecular Nanomachines at Work-A Neutron Spin Echo Study”
22 October 2009

Prof ROSSKY, Peter J
University of Texas at Austin, Texas, USA
“Coupling of Environmental and Electronic Dynamics in Excited State Relaxation”
29 June 2009

Prof SATO, Takaya
Department of Materials Engineering, Tsuruoka National College of Technology, Yamagata, Japan
“Novel Polyelectrolyte Membrane Using Polymer Brush Structure and Its Application to Lithium Ionic Battery”
27 March 2009

Dr SMIRNOV, Alexander V
Joint Institute for Nuclear Research, Russia
“Simulation of Laser Cooling Experiments at S-LSR”
2 February 2009
“Crystalline Ion Beams and the Ordered State of Ions”
10 February 2009

Prof SOLOSHONOK, Vadim A
Department of Chemistry and Biochemistry, The University of Oklahoma, Oklahoma, USA
“Self-Disproportionation of Enantiomers: A Manifesto”
22 May 2009

Research Fellow SONG, Jiangning
Monash University, Melbourne, Australia
“Characterizing Substrate Specificity of Proteases Using Machine Learning Techniques”
10 December 2009

Prof STRUNK, Christoph
Institute for Experimental and Applied Physics, University of Regensburg, Regensburg, Germany
“Carbon Nanotubes as a Playground for Quantum Physics: From Band Structure to Splitting Cooper Pairs”
25 May 2009

Prof TAGUCHI, Toshihiro
Department of Engineering, Setsunan University, Japan
“Computer Simulation of Laser Plasma”
26 August 2009

Dr TAKADA, Akihiko
Institute for Materials Chemistry and Engineering, Kyusyu University, Fukuoka, Japan
“Reology of Colloidal Dispersion System”
27 March 2009

Prof TANDON, Poonam
Department of Physics, University of Lucknow, India
“Vibrational Dynamics of a variety of Polymeric Structures”
18 December 2009

Assoc Prof VALIENTE, Gabriel
Technical University of Catalonia, Barcelona, Spain
“Alignment of Trees and Directed Acyclic Graphs in Computational Biology”
20 May 2009

Prof VALMALETTE, Jean-Christophe
Institut Matériaux Microélectronique et Nanosciences de Provence, Université du Sud Toulon Var, Toulon, France
“Which Structure for Very Small Nanoparticles?”
29 October 2009

Dr VERT, Jean-Philippe
Mines ParisTech, Institut Curie, INSERM U900, France
“Global Alignment of Protein-protein Interaction Networks by Graph Matching Methods”
6 July 2009

Prof WANG, Jianbo
Physical Organic and Synthetic Organic Chemistry, Peking University, Beijing, China
“Pd-Catalyzed Reaction of Diazo Compounds”
15 October 2009

Assist Prof WANG, Yong
Chinese Academy of Sciences, Beijing, China
“Probing the Regulatory Networks by Computational Models”
16 July 2009

“Probing the Organizational and Evolutionary Principles of Bio-Molecular Networks by Subnetworks”
10 December 2009

Prof WATANABE, Junji
Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, Japan
“Orientations of Polymer Liquid Crystals at Interfaces”
27 March 2009

Prof WU, Chi
Department of Chemistry and Department of Physics, The Chinese University of Hong Kong, China
“How Macromolecules Pass through a Nanopore”
1 May 2009

Assoc Prof WU, Lingyun
Chinese Academy of Sciences, Beijing, China
“Conditional Random Patternal Gorithm for LOH Inference and Segmentation”
10 December 2009

Dr YAMASHITA, Makoto
Daiichi Sankyo Company, Limited, Tokyo, Japan
“Drug Discovery for Influenza Antivirals”
13 March 2009

Dr YOSHIKAWA, Chiaki
International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Ibaraki, Japan
“Novel Biointerface: Size Exclusion Effect and Biocompatibility of Concentrated Polymer Brush”
27 March 2009

Dr ZHU, Shanfeng
Fudan University, China
“Enhancing MEDLINE Document Clustering by Incorporating MeSH Semantic Similarity”
2 February 2009

MEETINGS AND SYMPOSIA

**Next-Generation Supercomputer Project
“DDS Nano-Carrier: Micelle, Lipid Membrane, and Protein
Complex”**

Organized by OKAZAKI, Susumu; MATUBAYASI, Nobuyuki
29 January 2009 (Tokyo, Japan)

**Next-Generation Supercomputer Project
“Computational Molecular Science of Soft, Complex Systems”**

Organized by MATUBAYASI, Nobuyuki; OKAZAKI, Susumu
10 February 2009 (Kyoto, Japan)

The 5th Organoelement Chemistry Seminar

Organized by TOKITOH, Norihiro; SASAMORI, Takahiro;
MIZUHATA, Yoshiyuki
19–20 February 2009 (Kyoto, Japan)

International Symposium for Solution Chemistry

“Perspectives of Solution Chemistry: Present and Future”

Organized by IBUKI, Kazuyasu; KIMURA, Yoshifumi;
MATUBAYASI, Nobuyuki; WAKAI, Chihiro
27 June 2009 (Kyoto, Japan)

International Mini-workshop on “Hydration and ATP Energy”

Organized by MATUBAYASI, Nobuyuki; SUZUKI, Makoto
11 July 2009 (Kyoto, Japan)

CREST Symposium

**“International Symposium on Multi-Scale Dynamics of Protein
Complex Formation and Function”**

Organized by KITAO, Akio; TAKADA, Shoji; MATUBAYASI,
Nobuyuki; KUWATA, Kazuo
14-16 July 2009 (Tokyo, Japan)

**Kyoto University/Nagoya University/ Kyushu University Joint
Project of Chemical Synthesis Core Research Institutions,
“The 8th Forum on Material Synthesis”**

Organized by OZAWA, Fumiyuki
8 September 2009 (Kyoto, Japan)

**Kyoto University/Nagoya University/ Kyushu University Joint
Project of Chemical Synthesis Core Research Institutions,
“The 5th Symposium on Material Synthesis”**

Organized by OZAWA, Fumiyuki
19-20 November 2009 (Kyoto, Japan)

**“Japan-Taiwan Joint Symposium on New Functional Materials
and Their Nano-Scale Analysis”**

Organized by SHIMAKAWA, Yuichi
25-26 November 2009 (Kyoto, Japan)

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