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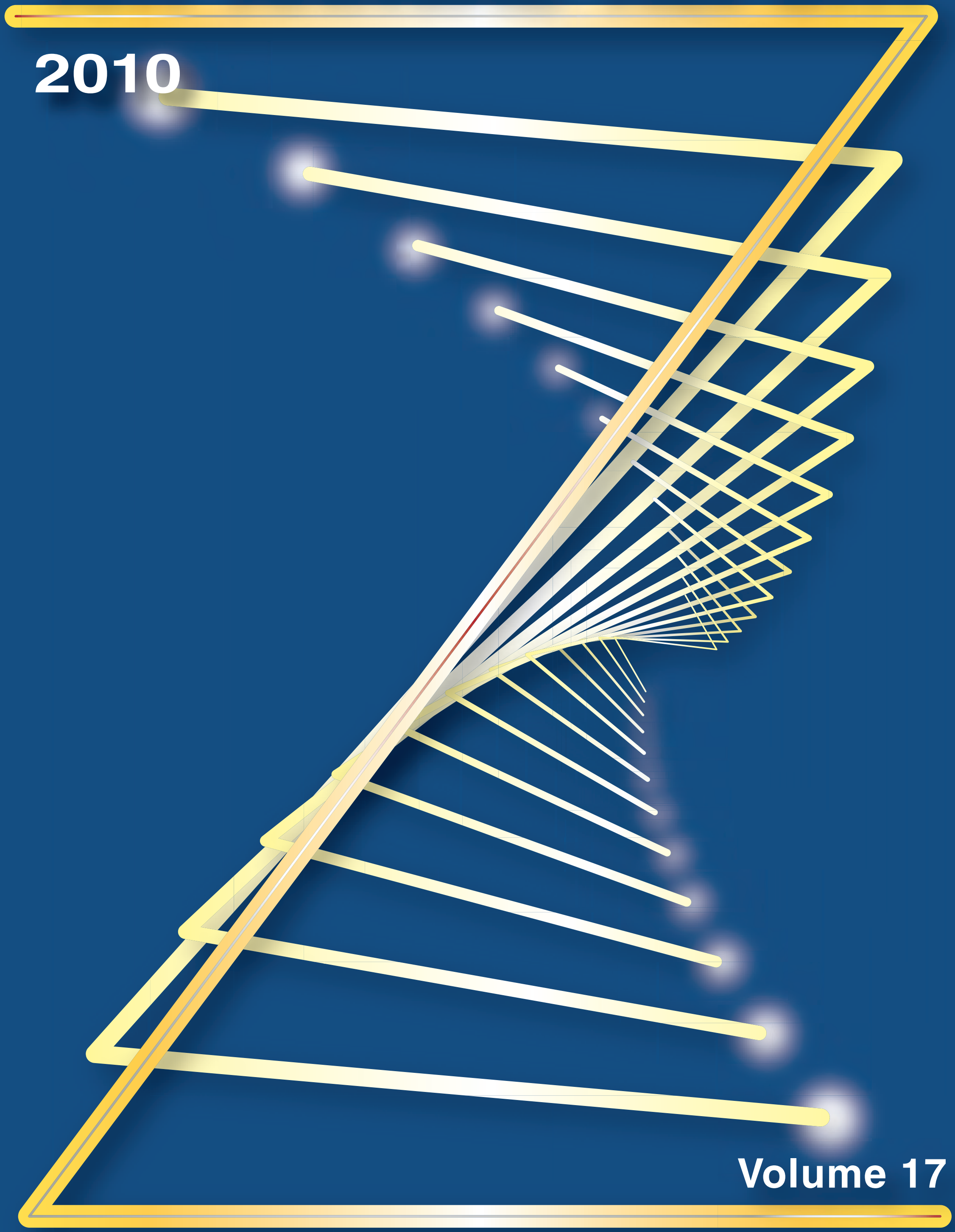
ICR ANNUAL REPORT

2010



Volume 17

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2010 (Volume 17) - ISSN 1342-0321 -

This Annual Report covers from 1 January to 31 December 2010

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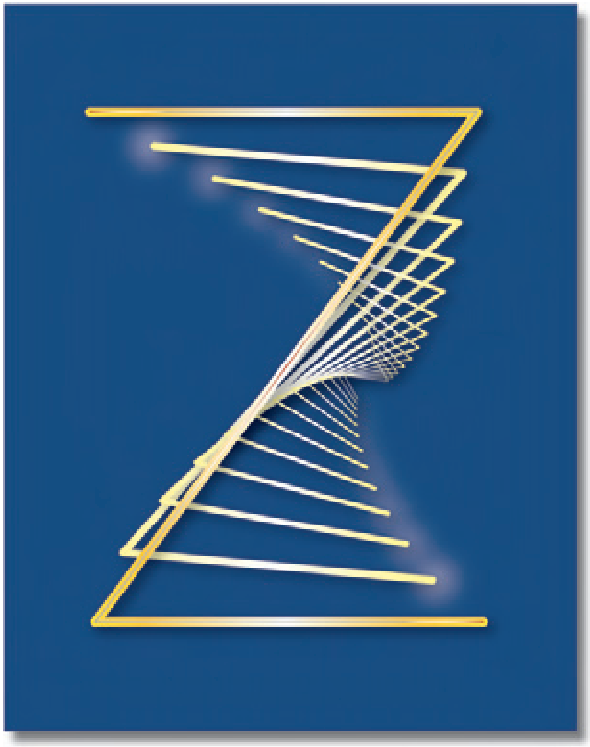


Institute for Chemical Research
Kyoto University
Volume 17

Preface

Institute for Chemical Research (ICR) dates back to 1915 with the founding of the Specialized Center for Chemical Research at the Faculty of Science, Kyoto Imperial University. The formation of the Specialized Center was greatly influenced by historical events. In 1910, Dr. Sahachiro Hata developed salvarsan, a highly effective drug for syphilis, while conducting research with Dr. Paul Ehrlich. The effectiveness of this compound eventually became widely recognized, and its commercial production began in Germany. Although Japan was importing this drug, the outbreak of the World War I ceased the importation, and forced by circumstances the Japanese government requested that the University of Tokyo and Kyoto University 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 basic principles of chemistry and their 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 32 research fields (laboratories) with 99 faculty members and about 240 graduate students. Each laboratory belongs to one of the seven graduate schools which encompass science, engineering, pharmaceutical science, 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 chemistry-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, the Graduate school of Science and Graduate school of Informatics. 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 Universality & 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 MEXT Project of Integrated Research on Chemical Synthesis (2010-2016)", in collaboration with the Catalysis Research Center at Hokkaido University, the Research Center for Materials Science at Nagoya University and the Institute for Materials Chemistry and Engineering at Kyushu University. This is the second stage of the project supported by MEXT through the Research and Education Funding for Inter-University Research Project. Furthermore, ICR is currently collaborating with domestic/oversea universities and research organizations (with 49 official international collaboration agreements) and has been functioning as a Joint Usage/Research Center supported by MEXT, "Frontier/Interdisciplinary Research Core in ICR for Deepening Investigation and Promoting Cooperation in Chemistry-Oriented Fields" (since 2010).

The strong 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. Fortunately, the four-year quakeproof renovation of the main buildings in Uji campus has just been completed at the end of 2010 together with the establishment of a new lecture hall "Uji Obaku Plaza" in 2009. With these highly improved research/education facilities, we are further activating ourselves to attain our founding philosophy. Thus, we respectfully request your continued support and encouragement.

January 2011

N. Tokitoh

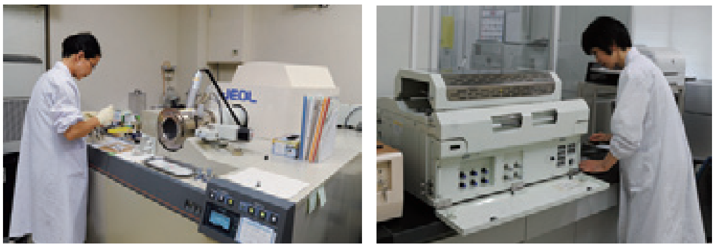
TOKITOH, Norihiro
Director

ICR News 2010

Joint Usage/Research Center: Frontier/Interdisciplinary Research Core in ICR for Deepening Investigation and Promoting Cooperation in Chemistry-Oriented Fields

Prof WATANABE, Hiroshi (Vice-Director of ICR)

Institute for Chemical Research (ICR) has been functioning, since April 2010, as the Joint Usage/Research Center (JURC) to deepen the investigation and promote the cooperation in chemistry-oriented fields. 68 joint research subjects have been adopted this year; please see p.67 for details. Several frontier instruments, including 800MHz Multi-purpose Nuclear Magnetic Resonance Spectrometer and Fourier Transform Ion Cyclotron Resonance Mass Spectrometer, have been newly equipped and utilized in the cooperative researches, and a management office for those common-use instruments has been also organized. The activity of JURC/ICR will bring a breakthrough into the global researches in the chemistry-oriented fields.



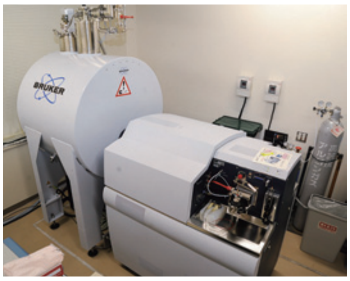
The management office for the common-use instruments

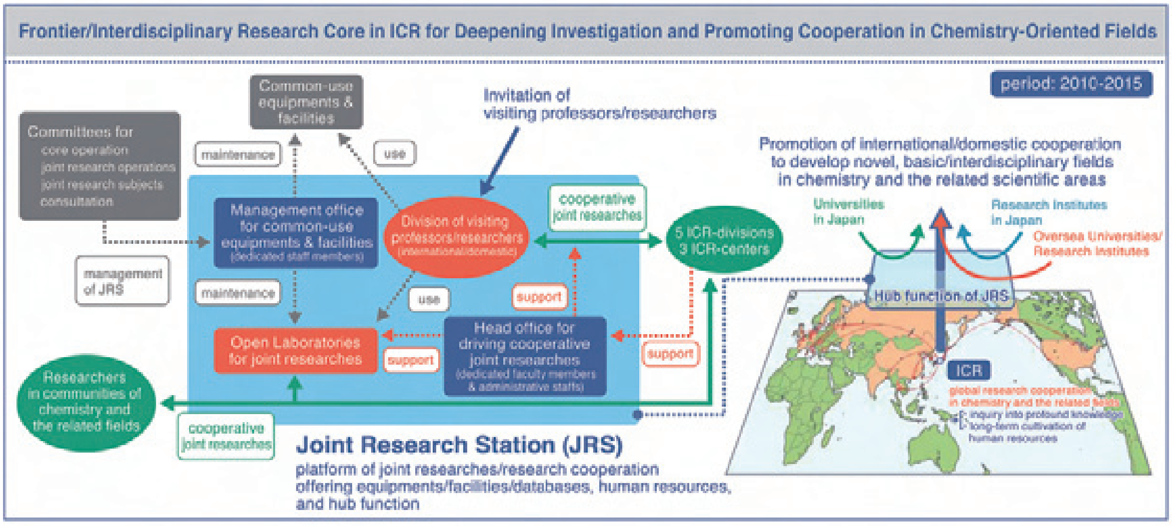
Versatile Super-High Field Nuclear Magnetic Resonance (NMR)

This 800 MHz NMR can be used both for solution- and solid-state measurements. 5 mmϕ multinuclear double-resonance probe, 5 mmϕ inverse detection triple-resonance probe, 10 mmϕ multinuclear double-resonance probe, triple-resonance CP/MAS probe, and high spinning speed CP/MAS probe are available.

Fourier Transform Ion Cyclotron Resonance Mass Spectrometer with 7.05 T Super Conducting Magnet (FT-ICR-Mass)

A Bruker Daltonics SolariX Qq-FT-ICR Mass Spectrometer, equipped with ESI, APCI, and MALDI ion sources with CID, ECD, and ETD fragmentation, enables ultra-high resolution (FWHM max >1,000,000) and ultra-high sensitivity (100 atmol) mass spectrometry measurements.

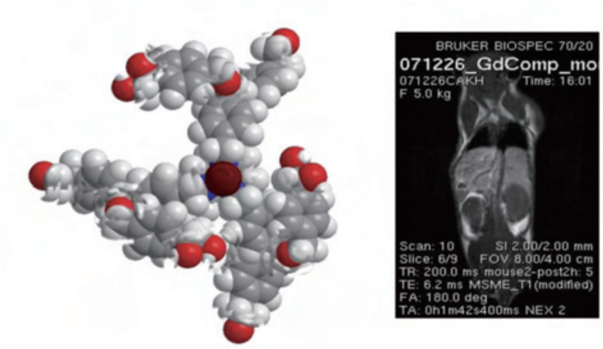




Division of Multidisciplinary Chemistry, Interdisciplinary Chemistry for Innovation (1 December 2010~)

Prof TOSHIMITSU, Akio

I feel it happy to come back to ICR, where I had been engaged in the research work for 30 years in the field of synthetic organic chemistry as an undergraduate and graduate student and as a researcher. I had been interested in asymmetric synthesis. In 2002, I moved to International Innovation Center to serve Kyoto University in the coordination of Industry-Academia partnership and in the application and license of intellectual properties. Recently my research interest has shifted to the design and synthesis of organic compounds which are attractive to industrial society from the viewpoint of innovation. The examples include pyrene derivatives used in light-emitting field-effect transistors, sugar-fullerene linked compounds used in photodynamic therapy of cancers, and gadolinium complex of chiral dendrimers used in magnetic resonance imaging of cancers (shown in the figure).



Gadolinium complex of chiral dendrimer (left) used in magnetic resonance imaging of cancer in mouse (right)

MEXT Project of Integrated Research on Chemical Synthesis (2010-2016)

Prof OZAWA, Fumiyuki (Director of IRCELS)

Organization

Elements Chemistry Research Station:
Institute for Chemical Research,
Kyoto University
Molecular Chemistry Research Station:
Research Center for Materials Science, Nagoya University
Assembly Chemistry Research Station:
Institute for Materials Chemistry and Engineering,
Kyushu University
Catalysis Chemistry Research Station:
Catalysis Research Center, Hokkaido University

The 1st Symposium on Material Synthesis
(3-4 December 2010, at Kyoto University)

A strong cooperative and collaborative research program will facilitate future advances in chemical synthesis. Our society expects innovative and highly functional materials. In order to respond to these demands, the education and training of young scientists would also benefit from a research environment that exposes them to different branches of materials chemistry. The purpose of this joint research program is to develop novel synthetic chemistry for production of new materials through the intimate cooperation of four highly recognized research groups. Examples of new materials and technologies that could arise from this research include: supramolecular organic electronics devices, metallic oxide nanoparticles, hydrogen production catalysts, electronic display device materials driven by structural control macromolecules, and hetero-atom conjugated materials with novel optical and electronic properties. These novel materials are expected to contribute to nano-science and materials science.

http://jointproject-cscri.rcms.nagoya-u.ac.jp/english/index.html

CONTENTS

Division of Synthetic Chemistry

Division of Materials Chemistry

Division of Biochemistry

Division of Environmental Chemistry

Division of Multidisciplinary Chemistry

Advanced Research Center for Beam Science

International Research Center for Elements Science

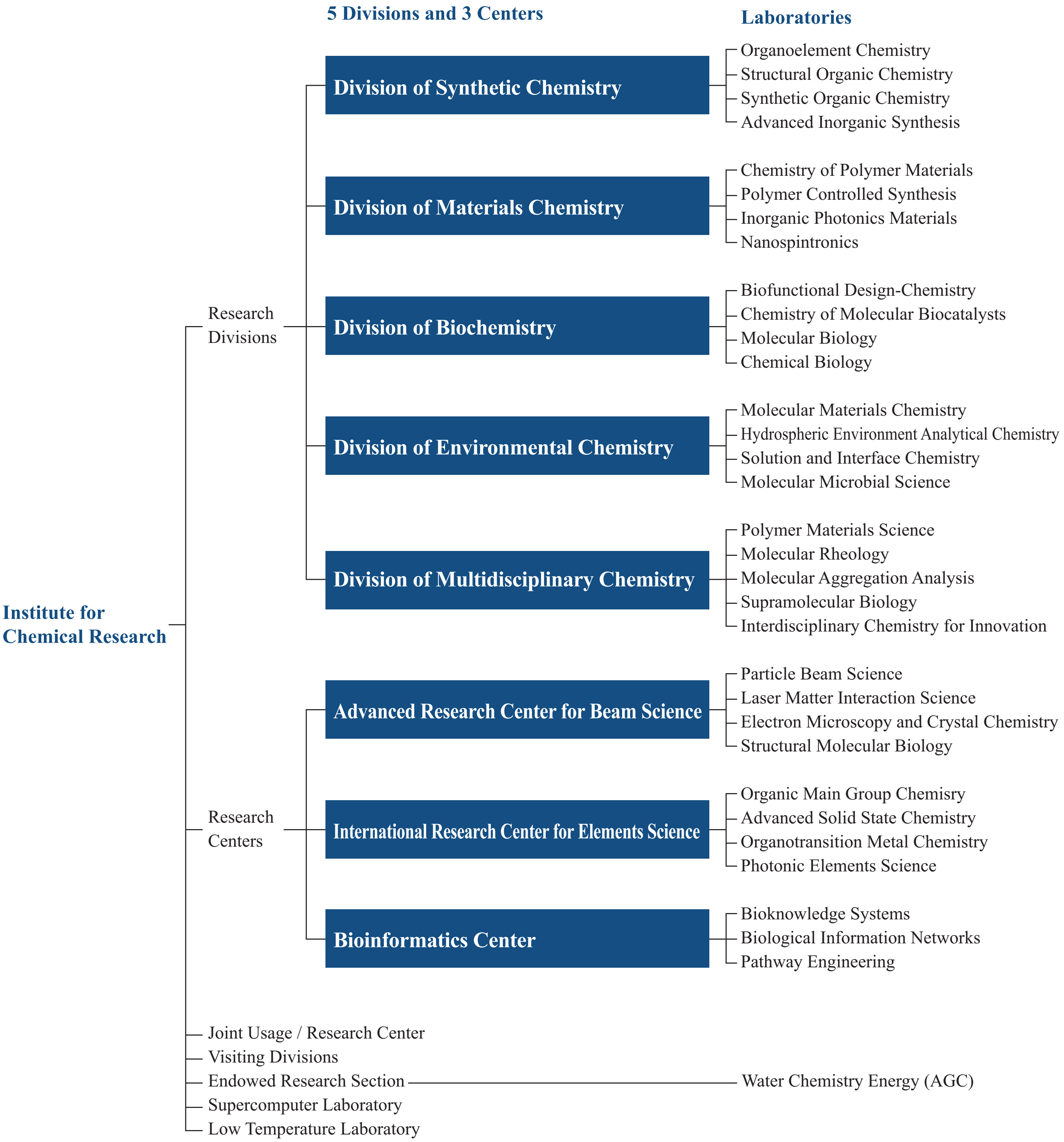
Bioinformatics Center

Endowed Research Section

Abbreviations used in the columns

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

ORGANIZATION



5 Divisions and 3 Centers

Laboratories

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

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry
– Organoelement Chemistry –

http://boc.kuicr.kyoto-u.ac.jp/www/index-e.html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TOKITOH, Norihiro
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TSURUSAKI, Akihiro
(D Sc)


PD
MIYAKE, Hideaki
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* Assist Prof of Pioneering Research Unit for Next Generation

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SATO, Takahiro (D2)
SUGAMATA, Koh (D2)
SAKAGAMI, Michiyasu (D1)
MIYAMOTO, Hisashi (M2)
NODA, Naoya (M2)
SHIMIZU, Tomohiro (M2)
EGAWA, Yasunobu (M1)

Visitors

Prof MUGESH, Govindasamy	Indian Institute of Science, India, 23–25 December 2009
Prof APELOIG, Yitzhak	Israel Institute of Technology, Israel, 23–25 April 2010
Prof ANG, How Ghee	Nanyang Technological University, Singapore, 9–10 December 2010

Scope of Research

KEYWORDS

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

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

Selected Publications

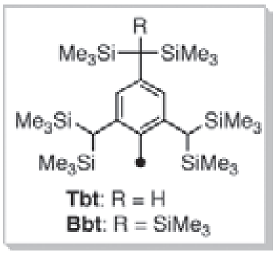
Han JS, Sasamori T, Mizuhata Y, Tokitoh N: Reactivity of an Aryl-Substituted Silicon—Silicon Triple Bond: Reactions of a 1,2-Diaryldisilyne with Alkenes, *J. Am. Chem. Soc.*, **132,** 2546-2547 (2010).

Sato T, Mizuhata Y, Tokitoh N: 1,2-Dialkynyldisilenes: Silicon Analogues of (*E*)-Enediyne, *Chem. Commun.*, **46,** 4402-4404 (2010).

Tsurusaki A, Nagahora N, Sasamori T, Matsuda K, Kanemitsu Y, Watanabe Y, Hosoi Y, Furukawa Y, Tokitoh N: Synthesis, Structures, and Reactivity of Kinetically Stabilized Anthryldiphosphene Derivatives, *Bull. Chem. Soc. Jpn.*, **83,** 456-478 (2010).

Tanabe Y, Mizuhata Y, Tokitoh N: Synthesis and Structure of a Heavier Congener of Biphenyl: 1,1'-Disila-4,4'-biphenyl, *Organometallics*, **29,** 721-723 (2010).

Characteristic Reactivity of a Diaryl-substituted Disilyne



Recently, we have reported the synthesis and isolation of the first stable 1,2-diaryldisilyne, Bbt–Si≡Si–Bbt, along with its unique properties. Reaction of the disilyne with alkenes afforded compounds having several unique skeletons depending on the kind of alkenes. Moreover, the disilyne showed high reactivity with alkynes, and both polar and non-polar alkynes reacted with it to give the corresponding 1,2-disilabenzenes as the major product. Crystal structure analysis showed that the central ring of the 1,2-disilabenzene was almost planar, and most notably, the Si–Si bond has significant *trans*-bent character. Evidence supporting its aromatic structure was collected by both experimental and theoretical means.

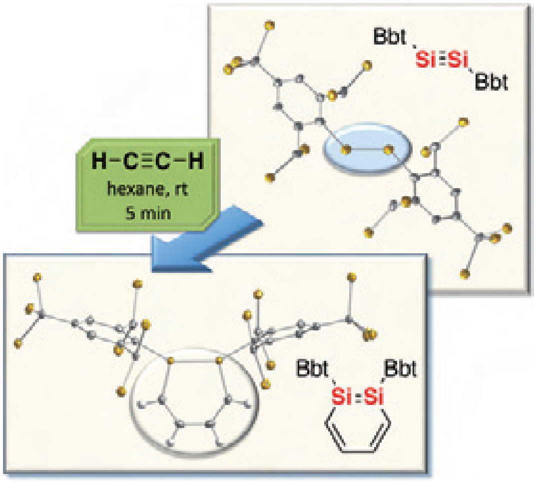


Figure 1. Generation of 1,2-Disilabenzene by the Reaction of a Disilyne with Acetylene.

Synthesis and Properties of 1,1'-Disila-4,4'-biphenyl

The 1,1′-disila-4,4′-biphenyl, the first molecule bearing directly connected two silaaromatic rings, was synthesized by utilizing the steric protection afforded by Tbt groups and characterized by its spectroscopic and X-ray crystallographic data. Its two SiC_5 rings are twisted with respect to each other with a dihedral angle of ca. 41º. The parent biphenyl has a coplanar structure due to packing forces in the crystalline state, and its dihedral angles in solution or in the gas phase are ca. 45º. In the case of the disilabiphenyl, extremely bulky Tbt groups prevent intermolecular interactions between the disilabiphenyl units, resulting in the retention of a distorted structure even in the solid state. Its UV-vis spectrum showed not only a red shift but also a 6-fold increase in absorbance of the longest absorption maximum in its electronic spectra in comparison with those of Tbt-substituted silabenzene, indicating that the concept of conjugation through the single bond connecting two aromatic rings is applicable even in the silaaromatic systems.

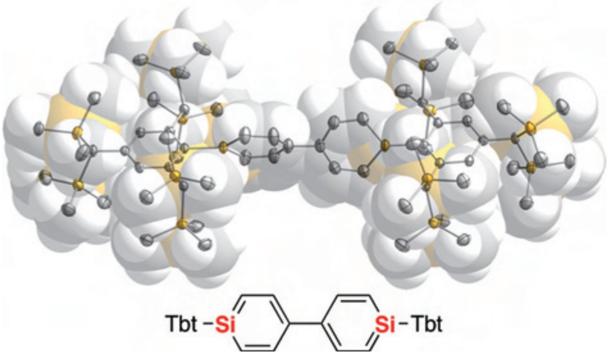


Figure 2. Structure of 1,1'-Disila-4,4'-biphenyl.

Synthesis and Properties of 1,2-Dialkynyldisilenes

Recently, several new disilene (>Si=Si<) systems have been designed and investigated to evaluate the conjugation between the Si=Si unit and the connected aryl sp^2-carbon conjugated systems. Although those disilenes exhibited optically and electrochemically unique properties, such π-conjugated systems are structurally limited. Therefore, the synthesis and isolation of the alkynyl-substituted disilenes, the silicon analogues of enediynes, are attractive from the viewpoint of elucidation of the conjugation between the Si=Si and sp-carbon units. We synthesized and isolated the first stable 1,2-dialkynyldisilenes and elucidated their structures using X-ray crystallography. In their UV/vis spectra, the absorption maximum of phenylethynyl-substituted disilene was more red-shifted than that of trimethylsilylethynyl-substituted one, indicating the π-conjugation between the Si=Si bond and phenyl groups through the C≡C bonds. Notwithstanding the different energy levels of p-orbitals between Si=Si and C≡C bonds, these findings showed that conjugation was possible between Si=Si and C≡C units.

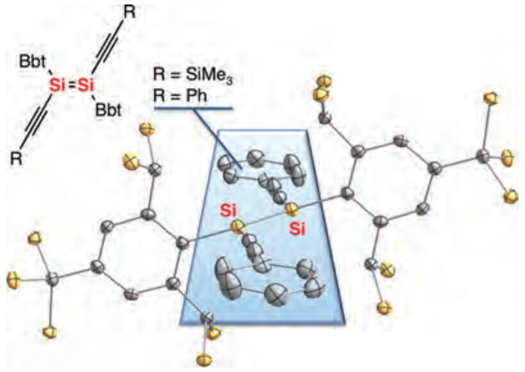


Figure 3. Structure of 1,2-Dialkynyldisilene.

Division of Synthetic Chemistry
– Structural Organic Chemistry –

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


Prof
MURATA, Yasujiro
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Assist Prof
MURATA, Michihisa
(D Eng)


PD
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(D Sc)


PD
TANIGUCHI, Takuhiro
(D Sc)

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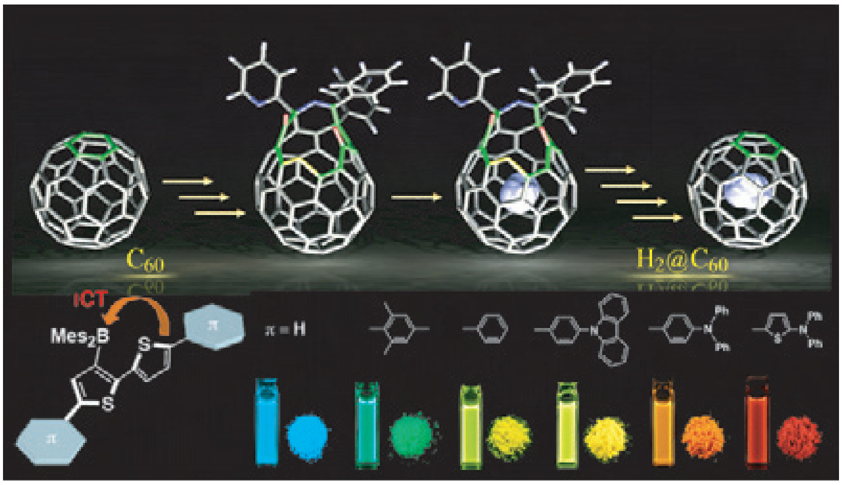
YASUI, Hidefumi (M2)
KATSUYA, Satoshi (M1)
NOBORI, Masahiro (M1)
NISHIMURA, Hidetaka (UG)
MORI, Haruki (UG)

Visitor

Prof DUNSCH, Lothar	Leibniz Institute for Solid State and Materials Research Dresden, Germany, 27 October
Prof GAN, Liangbing	Peking University, China, P. R., 29 October

Scope of Research

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



KEYWORDS
π-Conjugated Systems
Open-Cage Fullerenes
Endohedral Fullerenes
Functional Dyes
Organic Solar Cell

Selected Publications

Komatsu K, Murata M, Murata Y: Encapsulation of Molecular Hydrogen in Fullerene C_{60} by Organic Synthesis, *Science*, **307,** 238-240 (2005).

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

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

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

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

Rational Synthesis of Endohedral C_{60} and C_{70} Encapsulating a Helium Atom

Encapsulation of a molecule or atom in a small space with sub-nanometer size is currently attracting wide interests from the view point of basic science as well as storage purpose. Endohedral fullerenes encapsulating a small atom of rare gases such as helium, neon, argon, krypton, and xenon, are one of the most interesting systems among them. However, the generation of He@C_{60}, Ar@C_{60}, Kr@C_{60}, and Xe@C_{60} are so far relied on only high-pressure/high-temperature treatment (650 °C and 3000 atm or related conditions) of empty fullerenes, and the occupation levels thus obtained are limited to less than 1%. To study the intrinsic properties of such materials, it is necessary to synthesize them with high occupation levels. In this study, we present a rational synthesis of He@C_{60} and He@C_{70} by insertion of He into cage-opened fullerene derivatives followed by closure of the opening with keeping the encapsulated He inside the fullerene cages. The highest occupation levels for He@C_{60} (30%) and He@C_{70} (30%) were realized for the first time. Owing to the high occupation levels, enrichment of He@C_{60} and He@C_{70} became available, and more importantly, very weak interaction between the encapsulated He and fullerene cages were experimentally studied by ^{13}C NMR and HPLC.

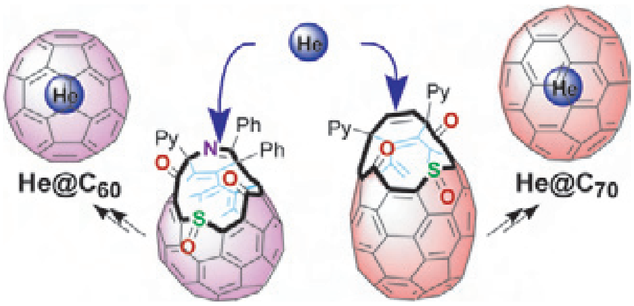


Figure 1. Synthesis of He@C_{60} and He@C_{70}.

Additon of Grignard Reagents to Open-Cage Fullerene Derivative

Research on fullerene derivatives with a large opening on the cage is of great significance in developing a new synthetic method to encapsulate a variety of atoms or molecules inside the cage. Actually, by synthesizing a cage-opened C_{60} derivative with a 13-membered-ring opening, we have demonstrated quantitative insertion of molecular hydrogen inside the cage through the opening and subsequent preparation of cage-closed C_{60} encapsulating H_2, i.e., H_2@C_{60}. In the present study, we have studied reactions of the cage-opened C_{60} derivative with Grignard reagents and shown that 1,2-addition selectively took place at one of the two carbonyl groups directly connected to the fullerenyl π-system at the opening. The resulting alcohol derivative was found to undergo transannular etherification under acidic conditions. In addition, electrochemical properties of the products were evaluated. The results shown in this study are useful to predict the reaction course of organometallic nucleophiles, such as Grignard reagents, to cage-opened fullerene derivatives with carbonyl groups.

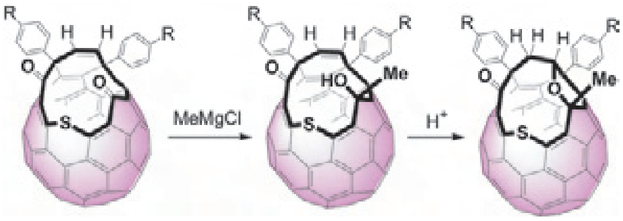


Figure 2. Reaction of the Open-cage C_{60} Derivative at the Rim of the Opening.

Electronic Tuning of Thiazolyl-Capped π-Systems

In the molecular design of π-conjugated materials, the modification of the electronic structure is an important issue to attain the required color absorption/emission, to facilitate the charge injection from electrodes, or to achieve ambipolar carrier transport, etc. On the other hand, C=N bond-containing π-conjugated systems, such as thiazole, are widely used skeletons for organic (opto)electronic materials owing to their inherent high electron affinity. As a new methodology for electronic modification of the C=N bond-containing π-electron systems, we disclosed electronic tuning of thiazolyl-capped π-conjugated compounds via a coordination/cyclization protocol with $B(C_6F_5)_3$. This electronic tuning protocol effectively enhances an electron-accepting character giving rise to lower reduction potentials and increases thermal stability.

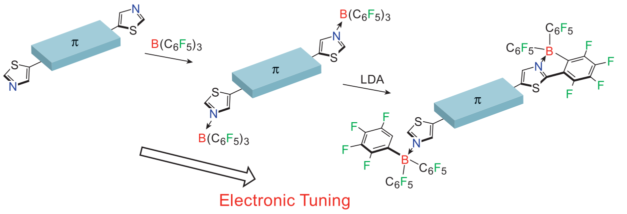


Figure 3. Electronic Tuning of Thiazolyl-Capped π-Conjugated Systems.

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Scope of Research

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

KEYWORDS

Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition

Selected Publications

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

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

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

Muramatsu W, Mishiro K, Ueda Y, Furuta T, Kawabata T: Perfectly Regioselective and Sequential Protection of Glucopyranosides, *Eur. J. Org. Chem.*, **5,** 827-831 (2010).

Functional Group Tolerance in Organocatalytic Regioselective Acylation of Carbohydrates

Organocatalytic regioselective acylation of mono- and disaccharides with various functionalized acid anhydrides has been developed. Acylation of octyl *β*-D-glucopyranoside with acid anhydrides derived from α–amino acids, cinnamic acid, and gallic acid took place at C(4)-OH in 78-94% regioselectivity in the presence of catalyst **1**. Especially, a disaccharide with seven free hydroxy groups (X=OH, R' =H) underwent acylation at C(4)-OH in 78% regioselectivity in the presence of **1**. The 4-*O*-acylates of the glucose moiety were universally obtained as the major acylate in the acylation of various carbohydrates with various functionalized acid anhydrides. The functional group tolerance in the regioselective acylation catalyzed by **1** was found to be high. This seems surprising because the hydrogen-bonding interactions (yellow rectangles) between C(6)- and C(3)-OH of the glucose moiety and the catalyst, which was proposed to be responsible for the selective 4-*O*-acylation, are supposed to be specifically operative even in the presence of many other hydrogen bond donors and acceptors (pink circles).

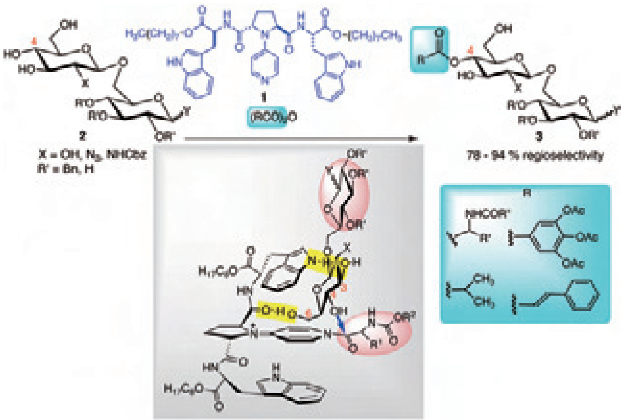

Figure 1. An organocatalytic regioselective acylation at C(4)-OH with functionalized acid anhydrides proceeds in the presence of other functional groups (pink circles) via specific hydrogen bonding interactions (yellow rectangles) between the catalyst and the substrates.

Perfectly Regioselective and Sequential Protection of Glucopyranosides

Regioselective manipulation of one of the multiple hydroxy groups of carbohydrates has been a fundamental challenge in organic synthesis. We have developed a perfectly regioselective and sequential method for the preparation of orthogonally protected glucopyranosides starting from alkyl and thioalkyl *β*-D-glucopyranosides. An acyl group was introduced at C(4)-OH by organocatalysis in >99% regioselectivity. TBDPS, Boc, and BOM groups were sequentially introduced into the 4-*O*-acyl-glucopyranoside at C(6)-OH, C(2)-OH, and C(3)-OH, respectively, in >99% regioselectivity in each step. Each of the protective groups (PG_1~PG_4) was readily removed to give the corresponding mono-ols with three different protective groups, which are possible intermediates for the synthesis of natural and modified oligosaccharides.

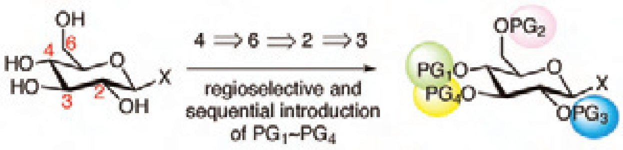

Figure 2. Preparation of an orthogonally protected glucose derivative by regioselective and sequential introduction of protective groups. An acyl group (PG_1) was introduced at C(4)-OH by organocatalyst **1** with >99% regioselectivity. TBDPS (PG_2), Boc (PG_3), and BOM (PG_4) groups were sequentially introduced at C(6)-OH, C(2)-OH, and C(3)-OH, respectively, in >99% regioselectivity and >98% yield in each step.

Axially Chiral Binaphthyl Surrogates with a Metal Center Directly Connected the Chiral C-N Axis

Chiral binaphthyls have been extensively used in asymmetric synthesis. In particular, metal complexes of 2,2'-disubstituted-1,1'-binaphthyls (**4**) have been shown to be extremely effective catalysts for a variety of asymmetric transformations. While the catalytically active metal center (M) in **4** is located far from the chiral axis (C(1)-C(1')) by three bonds, it is quite effective for asymmetric induction in many cases. The ultimate structure to minimize the distance between the metal center and the chiral axis is shown as **5** and **6** in which a metal center (Al) is directly connected to the chiral C(1')-X axis. X-ray analysis of **6** indicates that the complex adopts a conformation similar to that of 1,1'-binaphthyls. The racemization barrier of **5** was determined to be 23.0 kcal/mol, which was found to be higher by ~ 4 kcal/mol than the corresponding biaryl amine precursor with an N-H-N hydrogen bond.

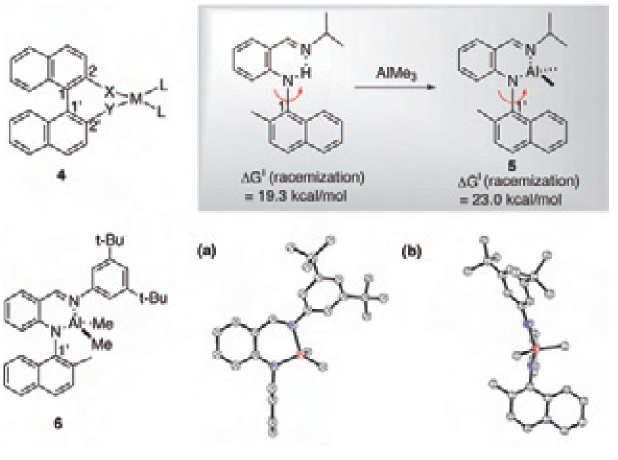

Figure 3. The racemization barrier of axially chiral binaphthyl surrogate **5** increased by ~4 kcal/mol compared to the corresponding biaryl amine precursor with an inner N-H-N hydrogen bond. (a) Top view (left) and (b) side view (right) of X-ray structure of **6**.

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Scope of Research

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

KEYWORDS

Precision Polymerization
Living Radical Polymerization
Polymer Brush
Hybrid Materials
Biointerface

Selected Publications

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

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Ohno K, Morinaga T, Koh K, Tsujii Y, Fukuda T: Synthesis of Monodisperse Silica Particles Coated with Well-Defined, High-Density Polymer Brushes by Surface-Initiated Atom Transfer Radical Polymerization, *Macromolecules*, **38,** 2137-2147 (2005).

Novel Gels of Bottle Brushes Synthesized by Living Radical Polymerization

Successful application of living radical polymerization (LRP) made it possible to fabricate well-defined “concentrated” polymer brushes (CPBs), where graft chains in a good solvent were highly stretched, giving properties quite different and unpredictable from those of semi-dilute polymer brushes (SDPB). One of the most interesting properties of CPBs is the super lubrication in solvents, which was reasonably ascribed to CPBs never mixing with each other at any high compressions for the conformational entropic reason of highly extended chains. Such demixing or non-interpenetrating interaction can be expected also for comb-like polymers, so-called bottle brushes, depending on side-chain length; with increasing chain length, the effective graft density at the outermost surface should decrease through a crossover in brush regime from CPB to SDPB. In order to demonstrate this, we have synthesized well-defined bottle brushes of polystyrene (PS) with a high side-chain density by LRP with a multi-functional initiator and crosslinking them by coupling between radicals at side-chain ends as illustrated in Figure 1. Frictional measurement using an atomic force microscope revealed that the lubrication property was much improved on the gel surface by decreasing the side-chain molecular weight from 5600 to 1300 (see Figure 1), as expected. We believe that these studies will open up a new route to precision surface modification.

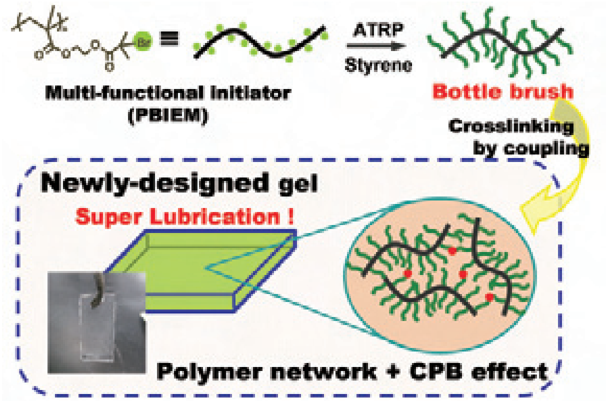

Figure 1. Synthesis of newly-designed gels of well-defined bottle brushes by LRP.

A Versatile Method of Initiator Fixation for Surface-Initiated Living Radical Polymerization on Polymeric Substrates

A facile yet robust approach to chemically fix an initiating group for atom transfer radical polymerization (ATRP) on various polymeric substrates was investigated. Conventional free radical copolymerization was conducted with methyl methacrylate (MMA), 2-(2-bromoisobutyryloxy)ethyl methacrylate (an ATRP initiator-carrying monomer, BIEM), and 2-((4-azidobenzoyl)oxy)ethyl methacrylate (a photoreactive phenylazide-carrying monomer, ABEM) in *N*,*N*-dimethylformamide at 75 °C, giving a random (statistical) copolymer (AIP). Thin films of the obtained copolymer were fabricated on poly(ethylene terephthalate) (PET) film surface by spin-casting a toluene solution of the terpolymer and were immobilized on the PET substrate via UV-irradiation using the photoreactivity of the phenylazido units. The surface-initiated ATRP (SI-ATRP) of poly(ethylene glycol) methacrylate (PEGMA) mediated by a copper complex was carried out in water at 30 °C in the presence of a sacrificial (free) initiator and the initiator-immobilized PET film as the solid substrate. The polymerization proceeded in a living fashion. The molecular weight of free polymer increased with polymerization time while retaining low-polydispersity index, and more importantly, the thickness of the poly(PEGMA) graft layer increased as a function of polymerization time with a reduced graft density (surface occupancy) as high as 0.5 in all examined time. This initiator immobilization technique was applied to various polymeric substrates including polystyrene, polypropylene, polyethylene, and polylactide. The fabrication of micropatterned polymer-brush surfaces was also demonstrated by photo-patterning the initiator layer followed by SI-ATRP.

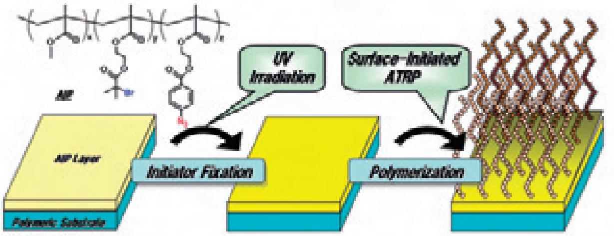

Figure 2. Chemical structure of phenyl azide- and atom transfer radical polymerization (ATRP) initiator-carrying random copolymer (AIP) and schematic representation for the immobilization of AIP on polymeric substrate followed by surface-initiated ATRP.

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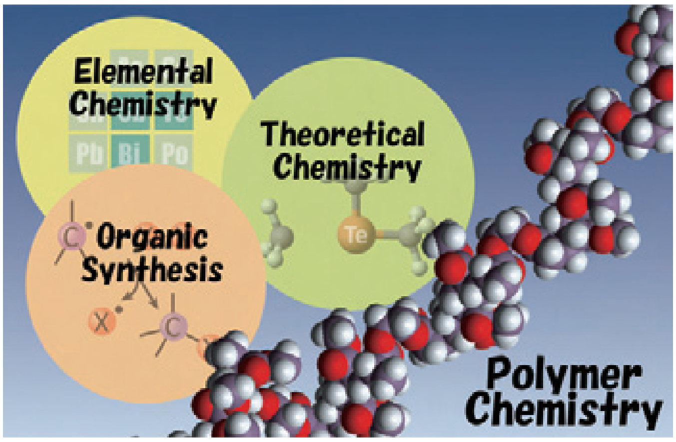
Scope of Research

Synthesis of structurally well-defined macromolecules has attracted great deal of attention, because such molecules would clarify structure-property relationship of polymers and lead to the development of new functional materials. Our research program focuses on development of new synthetic methods, which enable precise control of polymers and oligomers in terms of their size and structure. One such topic is the development of new living radical polymerization method utilizing heavier heteroatom compounds as controlling agents. The other topic is the synthesis of cycloparaphenylenes, hoop-shaped π-conjugated molecules, based on new synthetic strategy. We also study various polymer condensed states by both static and dynamic methods to understand the relation of physical properties and structures.



KEYWORDS

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

Selected Publications

Yamago S, Watanabe Y, Iwamoto T: Synthesis of [8]Cycloparaphenylene from a Square-Shaped Tetranuclear Platinum Complex [(cod)Pt(4,4'-biphenyl)]4, *Angew. Chem. Int. Ed.*, **49,** 757-759 (2010).

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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).

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Novel Synthetic Strategy of Cycloparaphenylenes

Cycloparaphenylenes are hoop-shaped π-conjugated molecules consisting from *p*-disubstituted benzene rings, and are the simplest structural unit of armchair carbon nanotubes. Due to their unique structure associated with expected unique properties, they have attracted the attention of various disciplines ranging from basic chemistry to material science. However, although they have a simple structure, their synthesis has been a significant challenge. We have succeeded in the selective synthesis of [8]cycloparaphenylene based on a new synthetic strategy (Figure 1).

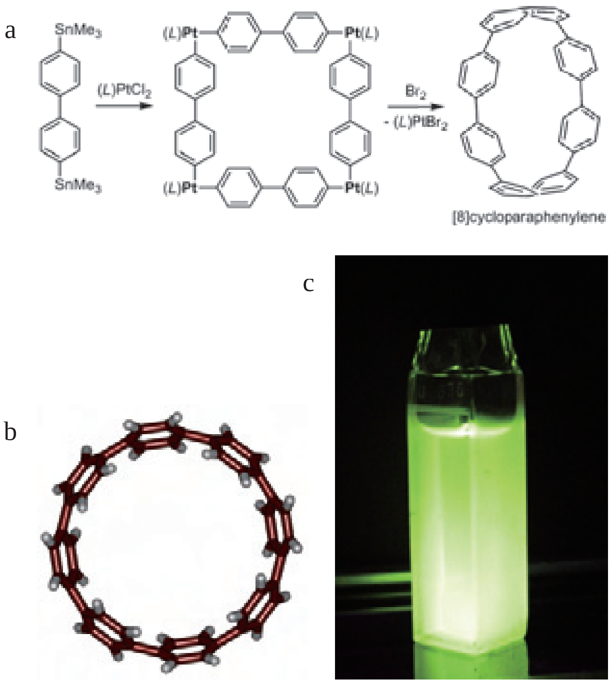


Figure 1. (a) Synthetic route, (b) computer-generated structure, and (c) luminescence of [8]cycloparaphenylene.

Hybrid Polymerization Method Mediated by Organotellurium Compounds

Living radical polymerization has become an indispensable method for the controlled synthesis of functionalized polymers, but applicability of this method is still limited to the certain class of vinyl monomers. We have already reported that organotellurium compounds are excellent controlling agents for living radical polymerization. Now we found that they also serve as efficient controlling agents for living cationic polymerization. Furthermore, living polymers, such as poly(meth)acrylates, prepared by organotellurium-mediated living radical polymerization were used for living cationic polymerization of vinyl ethers (Figure 2). This method enables access to new hybrid copolymers, which are difficult to synthesize by other methods.

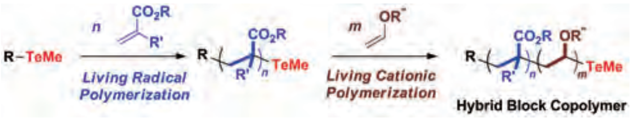
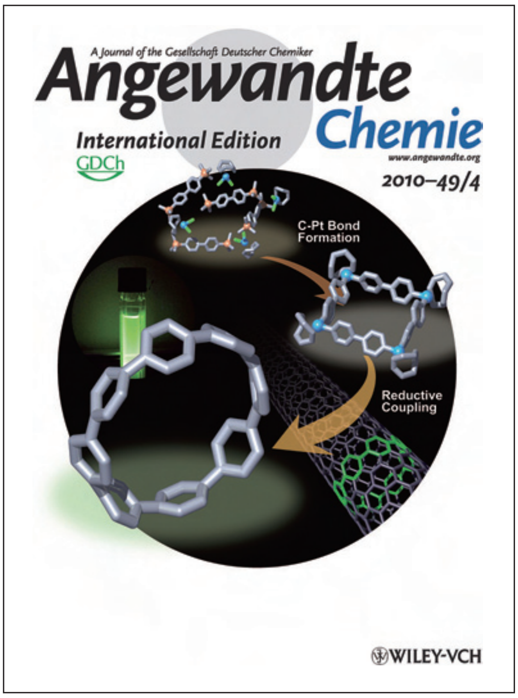


Figure 2. Synthesis of hybrid block copolymers by successive living radical and cationic polymerizations.



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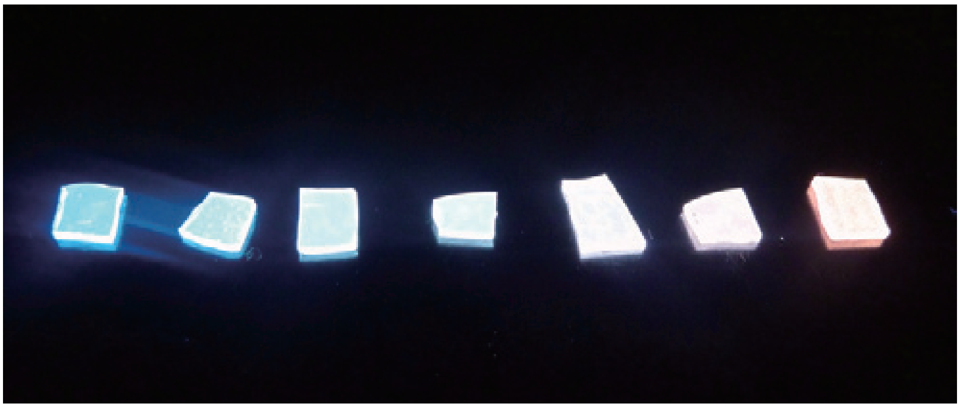
Scope of Research

In this laboratory, amorphous, polycrystalline inorganic materials and organic-inorganic hybrid materials with various optical functions such as photorefractivity, photolumionescence and photocatalysis are the target materials, which are synthesized by metathesis, 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.

KEYWORDS

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



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Masai H, Takahashi Y, Fujiwara T, Matsumoto S, Yoko T: High Photoluminescent Property of Low-Melting Sn-Doped Phosphate Glass, *Applied Physics Express*, **3,** 082102/1-082102/3 (2010).

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Menaa B, Takahashi M, Tokuda Y, Yoko T: Characterization and Solventless Growth of Salicylic Acid Macro-Crystals Involving a Nitrogen Gas Flow, *Cryst Res Tech.*, **45,** 341-346 (2010).

D-1 Structure Engineering of Organic-inorganic Hybrid Material by Solventless Synthesis

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 process. However, the sol-gel process is sometimes complicated, and it is difficult to obtain a monolith because of the crack formation during solvent evaporation.

Recently, another synthesis route for organic-inorganic hybrids, involving solventless reactions using orthophosphoric acid and organically modified silanes, has been developed. In this process the following metathesis occurs on heating: Si–X + P–OH $\rightarrow$ Si–O–P + HX$\uparrow$ (X = Cl, ethoxy), where groups that do not participate in this reaction are omitted from the reaction formula. This reaction proceeds with eliminations of HX because the reaction temperature is near/above the boiling point of HX. Because of the absence of solvent evaporation, a transparent, crack-free, large, hybrid monolith can be produced simply by mixing the starting reagents, followed by heat-treatment.

We have developed a new class of proton-conducting organic–inorganic hybrid silicophosphite membranes, produced by ethanol condensation under solventless and one-pot conditions. The membranes exhibit good thermal stability up to intermediate temperatures (~218 °C). Structural analyses using ^{29}Si and ^{31}P NMR spectroscopy and IR measurements have revealed that ethanol condensation produced an inorganic alternating copolymer structure, Si–O–P, with a phosphole group, and successive polymerization enabled these structures to connect with each other. In this way, it is possible to achieve structure engineering of inorganic–organic networks. The proton conductivities of the hybrids are as high as 5.2×10^{-3} S cm^{-1} at 85 °C under 80% relative humidity.

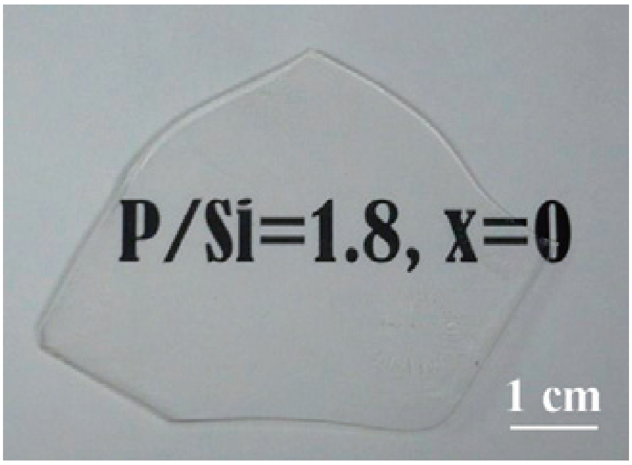

Figure 1. Photograph of an organic-inorganic hybrid phosphosilicate membrane. Crack-free and large-sized membranes can be prepared.

D-2 Fabrication of Rare Earth Free White Glass Phosphor

Recently, the three-band lamps consisting of rare earth (RE)-doped blue, red, and green phosphors and the white light emitting diode (LED) basically consisting of blue-LED and yellow phosphor, such as $Y_3Al_5O_{12}$:Ce^{3+} have been commercially available. However, these white emitting devices consisting of sharp emission bands possess lower colour rendering than the conventional broad band emission device. In addition, RE-free material will be required from a view point of uneven distribution of RE on earth. Here, our group has emphasized that white emission constituted of various kinds of wavelength can be attained by RE-free phosphor, such as Sb^{3+},Mn^{2+}-doped calcium halophosphate, ($Ca_5(PO_4)_3(F,Cl)$:Sb^{3+},Mn^{2+}). Although the emission of the calcium halophosphate possesses two broad emission bands, these emission bands are inherently fixed because of the crystal structure. On the other hand, it is more hopeful that amorphous oxide glass material will show white light without RE cation, because it is possible to tune the various coordination fields of the emission centre. If a glass material without RE cation shows the high emission property comparable to the crystalline phosphor, it will become a novel emitting material possessing wide chemical composition or good formability that can be applied to the industrial manufacturing. Such an emitting material is quite different from the conventional RE-doped crystalline phosphor. Recently, we have succeeded in preparing the Sn-doped transparent glass possessing high quantum efficiency ever reported. Our group is aiming at developing a novel white glass phosphor for UV LED.

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ARAKAWA, Tomonori (M2)
NISHIHARA, Yoshitaka (M1)
HIRAMATSU, Ryo (M1)

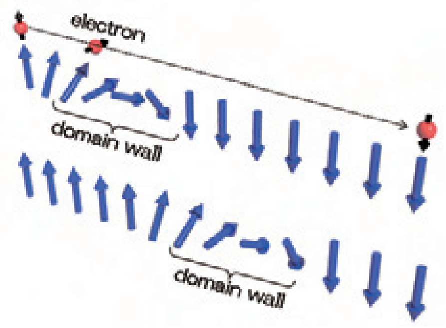
Visitor

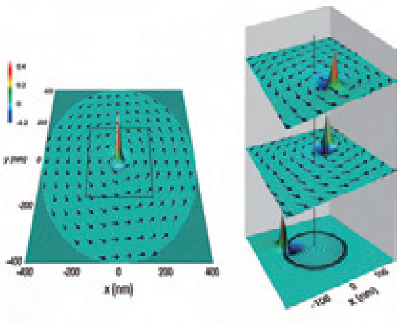
Prof WULFHEKEL, Wulf	Karlsruhe University, Germany, 25 October–4 December

Scope of Research

KEYWORDS
Spintronics
Quantum Transport
Nano-fabrication
Artificial Materials

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 nano-fabrication, we focus on the development of spin properties of various materials and the control of quantum effects in mesoscopic systems for novel spintronics devices.





Selected Publications

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

Kasai S, Nakatani Y, Kobayashi K, Kohno H, Ono T: Current-driven Resonant Excitation of Magnetic Vortex, *Physical Review Letters*, **97,** [107204-1]-[107204-4] (2006).

Yamada K, Kasai S, Nakatani Y, Kobayashi K, Kohno H, Thiaville A, Ono T: Electrical Switching of the Vortex Core in a Magnetic Disk, *Nature Materials*, **6,** 269–273 (2007).

Tanigawa H, Kondou K, Koyama T, Nakano K, Kasai S, Ohshima N, Fukami S, Ishiwata N, Ono T: Current-driven Domain Wall Motion in CoCrPt Wires with Perpendicular Magnetic Anisotropy, *Applied Physics Express*, **1,** [011301-1]-[011301-3] (2008).

Delmo MP, Yamamoto S, Kasai S, Ono T, Kobayashi K: Large Positive Magnetoresistive Effect in Silicon Induced by The Space-Charge Effect, *Nature*, **457,** 1112–1115 (2009).

Nakamura S, Yamauchi Y, Hashisaka M, Chida K, Kobayashi K, Ono T, Leturcq R, Ensslin K, Saito K, Utsumi Y, Gossard AC: Nonequilibrium Fluctuation Relations in a Quantum Coherent Conductor, *Physical Review Letters*, **104,** [080602-1]-[080602-4] (2010).

Spin-wave Manipulation

Spin-wave-based devices for signal processing have been of great interest for the spintronic integrated circuits in virtue of ultrafast propagation and low power consumption. In FeNi film, the magnetostatic surface wave (MSSW) is the promising mode due to its large propagation velocity and a nonreciprocal character which was also observed a long time ago in yttrium iron garnet films. We demonstrate the nonreciprocal emission of spin-wave packet in FeNi thin film in time domain. We show that the amplitude of spin wave depends on the direction of magnetization and that the phase of spin wave can be controlled by the polarity of pulsed magnetic field for the excitation. Our findings lead to the simple method of logical inputs of "1"/"0" into the spin-wave logic circuit.

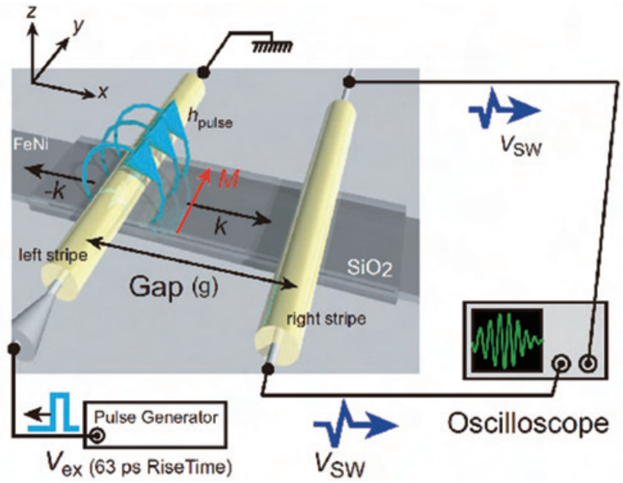


Figure 1. Schematic of time-resolved measurements of spin wave packet. A spin wave packet is generated and detected with a pair of asymmetric coplanar stripe with a gap.

Fluctuation Theorem in Quantum Regime

The linear-response theory, which is one of the triumphs in physics, was proposed in 1950’s. Triggered by Einstein’s work on the Brownian motion followed by the Johnson-Nyquist relation in an electrical circuit, the fluctuation-dissipation relation has been developed into the linear-response theory, which successfully relates a macroscopic irreversible process with underlying microscopic reversible equation of motion. The theory is now well-established as a standard tool to quantitatively predict the response of a variety of physical systems, and constitutes a reliable foundation in a wide range of physics, especially in statistical physics and condensed-matter physics. However, it is only justified very close to the equilibrium, and therefore an intensive attempt to expand the theory to non-equilibrium regime has been conducted for about half a century. In 1990’s, the fluctuation theorem (FT), which is validated even far from equilibrium, was discovered. While there is an experimental demonstration of its validity in a classical regime, the validity of FT in the quantum regime was left to be addressed. We experimentally demonstrate the presence of higher-order correlations between the current and the current noise in a mesoscopic electron interferometer, which corresponds to the next order correlation following to the Johnson-Nyquist relation. Our results qualitatively validate the predictions based on FT, being the first experimental evidence of FT in the non-equilibrium quantum regime.

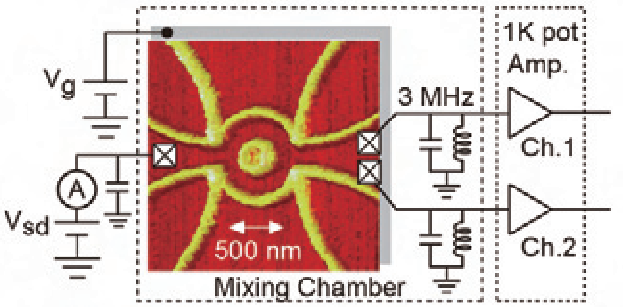


Figure 2. The atomic force microscope image of the mesoscopic electron interferometer, where our experimental test of FT was performed. The measurement setup is schematically shown.

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– Biofunctional Design-Chemistry –

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Prof
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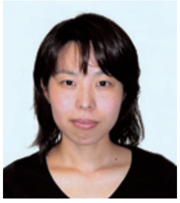
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Assist Prof
NAKASE, Ikuhiko
(D Pharm Sc)


PD
TANAKA, Gen
(D Eng)


PD
PUJALS, Sílvia
(Ph D)

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NOSHIRO, Daisuke (D2)
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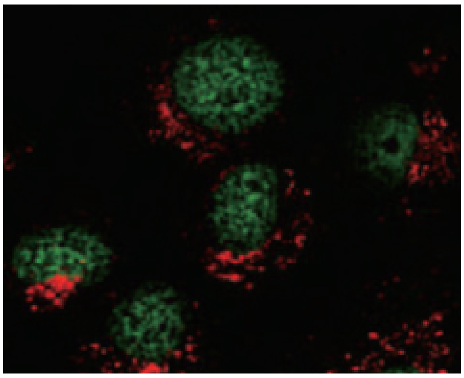
NOGUCHI, Haruka (M2)
OKUMURA, Shinya (M2)
TAKAYAMA, Shota (M2)
TSUDA, Nami (M2)
IMAI, Haruka (M1)
MIYAMAE, Hiroki (M1)
YAMAMOTO, Kazutoshi (M1)
MASUI, Ryosuke (UG)
MATSUMURA, Kazushi (UG)
OKU, Akihiko (UG)

Visitors

Prof GARIÉPY, Jean	Department of Medical Biophysics, University of Toronto, Princess Margaret Hospital, Ontario Cancer Institute, Canada, 24 August
Prof GRÄSLUND, Astrid	Department of Biochemistry and Biophysics, Stockholm University, Sweden, 2 November
FATEMEH, Madani	Department of Biochemistry and Biophysics, Stockholm University, Sweden, 2 November
Dr LINDBERG, Staffan	Department of Neurochemistry, Stockholm University, Sweden, 2 November
Prof GIRALT, Ernest	Institute for Research in Biomedicine Parc Cientific de Barcelona, Spain, 2–13 December

Scope of Research

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



KEYWORDS
Membrane-Permeable Peptides
Intracellular Delivery
Peptide Design
Zinc Finger Protein

Selected Publications

Yu HH, Nakase I, Pujals S, Hirose H, Tanaka G, Katayama S, Imanishi M, Futaki S: Expressed Protein Ligation for the Preparation of Fusion Proteins with Cell Penetrating Peptides for Endotoxin Removal and Intracellular Delivery, *Biochim Biophys Acta*, **1798,** 2249-2257 (2010).
Noshiro D, Asami K, Futaki S: Metal-assisted Channel Stabilization: Disposition of a Single Histidine on the N-terminus of Alamethicin Yields Channels with Extraordinarily Long Lifetimes, *Biophys J*, **98,** 1801-1808 (2010).
Nakase I, Kobayashi S, Futaki S: Endosome-disruptive Peptides for Improving Cytosolic Delivery of Bioactive Macromolecules, *Biopolymers*, **94,** 763-770 (2010).
Imanishi M, Nakaya T, Morisaki T, Noshiro D, Futaki S, Sugiura Y: Metal-stimulated Regulation of Transcription by an Artificial Zinc-finger Protein, *Chembiochem*, **11,** 1653-1655 (2010).

Metal-Assisted Channel Stabilization: Disposition of a Single Histidine on the N-terminus of Alamethicin Yields Channels with Extraordinarily Long Lifetimes

Alamethicin, a member of the peptaibol family of antibiotics, is a typical channel-forming peptide with a helical structure. The self-assembly of the peptide in the membranes yields voltage-dependent channels. The channels are characterized by frequent fluctuation of several current levels due to spontaneous uptake and release of alamethicin molecules into/from the channel assembly. Because certain classes of biological ion channels, including the nicotinic acetylcholine receptor (nAChR), have parallel bundles of amphipathic α-helices around the channel pores, alamethicin has been studied as a simplified model of such channel proteins and has been employed as an appropriate framework for creating artificial ion channels. In this study, three alamethicin analogs possessing a charged residue (His, Lys or Glu) on their N-termini were designed with the expectation of stabilizing the transmembrane structure (Figure 1). A slight elongation of channel lifetime was observed for the Lys and Glu analogs. On the other hand, extensive stabilization of certain channel open states was observed for the His analog. This stabilization was predominantly observed in the presence of metal ions such as Zn^{II}, suggesting that metal coordination with His facilitates the formation of a supramolecular assembly in the membranes. Channel stability was greatly diminished by acetylation of the N-terminal amino group, indicating that the N-terminal amino group also plays an important role in metal coordination. In addition, the potential applicability of the His analog channel to metal sensing was also demonstrated.

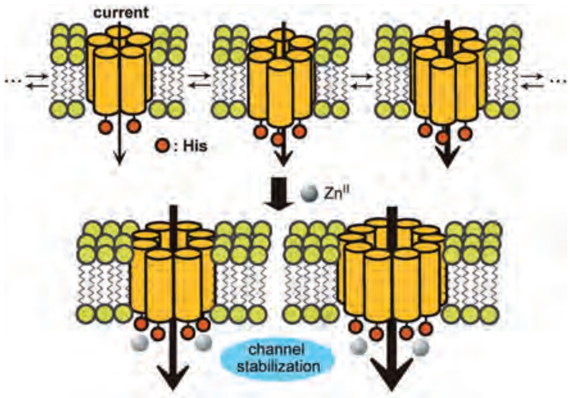


Figure 1. Schematic representation of channel formation of the His analog of alamethicin in the membrane.

Metal-Stimulated Regulation of Transcription by an Artificial Zinc-Finger Protein

The regulation of the gene expression of specific genes at a desired time opens attractive avenues for research in chemical biology, cell biology, and future gene therapy. A C2H2-type zinc finger motif, one of the most ubiquitous DNA binding motifs, binds a zinc ion with two conserved cysteine (Cys: C) and two histidine (His: H) residues. Zn^{II} binding is necessary for the proper folding of the peptides into the globular $\beta\beta\alpha$ structure and for the DNA binding ability. The binding between a typical C2H2-type zinc finger peptide and Zn^{II} is extremely stable. Such C2H2-type zinc fingers always preserve the Zn^{II} ions inside the cells and thus, it is difficult to control their DNA binding ability by changing the Zn^{II} concentration. By substituting zinc-ligating residue(s) of a C2H2-type zinc finger motif, we expected that the binding affinity to Zn^{II} would decrease and that the DNA binding ability of the peptide can eventually be controlled by changes in the Zn^{II} concentration (Figure 2). By substituting zinc-ligating residue(s) to CDH2-type, we succeeded in controlling the DNA binding and transcriptional ability of the peptide in response to changes in the Zn^{II} concentration. This zinc finger-based system has the bright prospect of an important prototype for the design of metal-responsive artificial transcriptional switches.

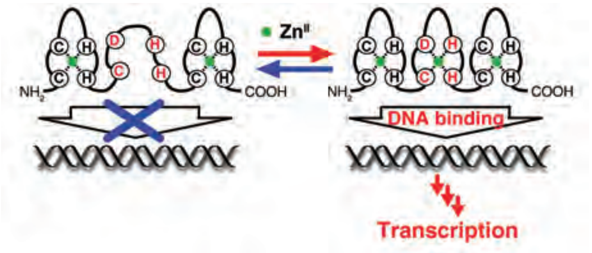


Figure 2. Zn(II) concentration responsive DNA binding of a ligand substituted zinc finger protein, CDH2-ZF3.

Division of Biochemistry
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WATANABE, Bunta
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OTOKAWA, Takuya (M2)
TABUCHI, Yukiko (M2)
YAMAMOTO, Yuki (M2)
MORI, Kohei (M1)
MORIKITA, Tatsuya (M1)

Scope of Research

Our research interests are the molecular design and synthesis of specific inhibitors of physiologically important enzymes (biocatalysts) for use as chemical probes to understand the reaction mechanisms, three-dimensional structures and physiological roles of the enzymes. The finely designed inhibitors are further elaborated to develop useful *in vivo* active biochemical reagents and the lead compounds for pharmaceuticals and agrochemicals. Our current research includes the design, synthesis and applications of transition-state analog and mechanism-based inhibitors of the key enzymes in glutathione homeostasis, asparagine synthesis, and the acyl-activating enzyme superfamily that plays pivotal roles in plant hormone homeostasis, secondary metabolite biosynthesis and β-oxidation of fatty acids. The synthesis and evaluation of substrates and inhibitors of ABC transporters and the unique enzymes of Archaea hyperthermophiles are also studied.

KEYWORDS

Enzyme Reaction Mechanisms
Transition-State Analog Inhibitors
Mechanism-Based Inhibitors
Glutathione
Chemotherapeutic Agents

Selected Publications

Ikeuchi Y, 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).

Hiratake J: Novel Inhibitor of γ-Glutamyl Transpeptidase (GGT): Unique Chemical Tools to Probe the Physiological Significance of GGT, *Wako Chemicals Jihou*, **76 (No. 3),** 2–6 (2008) (in Japanese).

Han L, Hiratake J, Kamiyama A, Sakata K: Design, Synthesis and Evaluation of γ-Phosphono Diester Analogues of Glutamate as Highly Potent Inhibitors and Active Site Probes of γ-Glutamyl Transpeptidase, *Biochemistry*, **46,** 1432–1447 (2007).

Guitierrez JA, Pan Y.-X, Koroniak L, Hiratake J, Kilberg MS, Richards NGJ: An Inhibitor of Human Asparagine Synthetase Suppresses Proliferation of an L-Asparaginase Resistant Leukemia Cell Line, *Chem. Biol.*, **13,** 1339–1347 (2006).

Nakatsu T, Ichiyama S, Hiratake J, Saldanha A, Kobayashi, N, Sakata K, Kato H: Structural Basis for Spectral Difference in Luciferase Bioluminescence, *Nature*, **440,** 372–376 (2006).

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

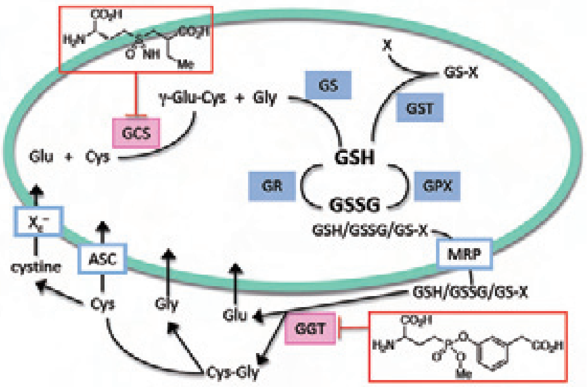


Figure 1. Biosynthesis, reaction and metabolism of glutathione (GSH) in cell. The specific inhibitors of GCS and GGT are shown (red squares).

Glutathione (GSH, γ-Glu-Cys-Gly) is an ubiquitous tripeptide found in many organisms, and plays central roles in the redox status of cells not only by detoxification of reactive oxygen species, but also by regulating the transcription of specific genes such as phase II anti-oxidant enzymes. We are interested in regulating the cellular GSH level that leads to the modulation of cellular redox status by controlling the activities of its biosynthetic enzyme, γ-glutamylcysteine synthetase (GCS), and its metabolic enzyme, γ-glutamyl transpeptidase (GGT), by using specific inhibitors (Figure 1). The compound **1**, designed as a transition-state analog, was found to serve as a potent mechanism-based inhibitor of GCS. The X-ray crystal structure of *E. coli* GCS in complex with **1** (Figure 2) revealed that the carboxy group (blue) as well as the side chain (magenta) is critical for the recognition by GCS, thereby the inhibition potency of **1** being 500-times higher than a classical GCS inhibitor, BSO, lacking the carboxy group. Furthermore, the introduction of a cyano group (compound **2**) as a mimic of SH further increased the inhibition potency by 31 and 55 times for the *E. coli* and the pathogenic *Streptococcus agalactiae* GCS, respectively. Notably, the inhibition potency of **2** is significantly higher (10,000 times) than BSO for the latter enzyme. The negatively charged carboxy group, however, appears to hinder the penetration of **1** and **2** through the cell membrane. Therefore a series of dipeptide-based inhibitors **3** was prepared for active transport through bacterial peptide transporters. This aspect of study is now under way to develop novel pharmaceuticals to combat multi-drug resistant pathogenic bacteria.

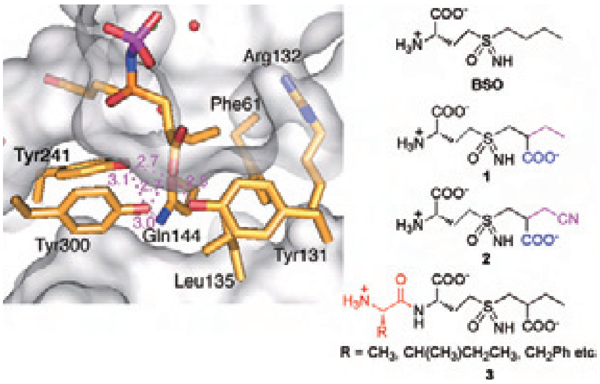
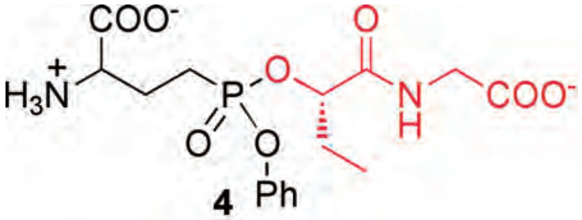


Figure 2. X-Ray crystal structure of the Cys binding site of *E. coli* GCS in complex with **1**.

In glutathione biosynthesis, another limiting factor is the availability of Cys. γ-Glutamyl transpeptidase (GGT) is a key enzyme in supplying the cells with Cys by cleaving the γ-glutamyl bond of GSH, as well as in degrading GSH conjugates for detoxification. We have developed a series of phosphonate-based inactivators of GGT and found that a glutathione-like inhibitor **4** was highly efficient for human GGT. In light of the specific recognition of the C-terminal carboxy group by human GGT, a simplified peptide analog **5** was prepared and found to be a highly potent inactivator of human GGT. The inhibitor **5** was specific for GGT, non-toxic and rather stable compound, serving as a useful biochemical reagent to knock down GGT *in vivo*. Interestingly, compound **5** significantly increased the biosynthesis of collagen I of human skin fibroblasts and can be used, for example, as a novel anti-aging cosmetic ingredient.



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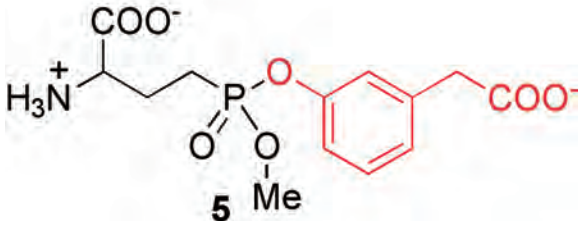

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Division of Biochemistry
– Molecular Biology –

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TSUGE, Tomohiko
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Res
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NAKAI, Hideto (D3)
WADA, Yukika (D1)
ANZAI, Naoko (M2)

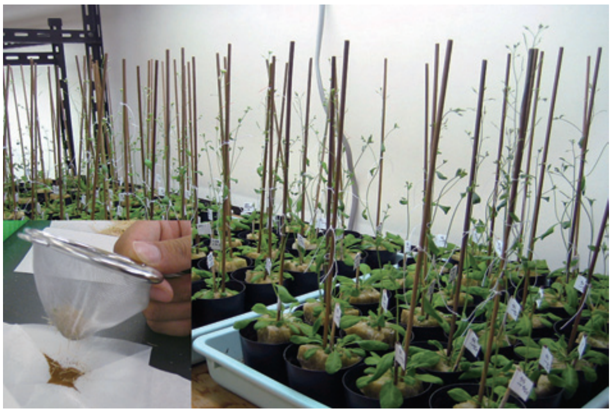
Visitors

Prof QU, Li-Jia	College of Life Science, Peking University, China, P.R., 11–14 December 2010
Ms LUO, Yu	College of Life Science, Peking University, China, P.R., 6 October 2010–31 October 2011
Ms WEI, Jia	College of Life Science, Peking University, China, P.R., 6 October 2010–31 October 2011

Scope of Research

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

KEYWORDS
Morphogenesis
Signal Transduction
Phospholipid
COP9 Signalosome
Cytokinin



Selected Publications

Taniguchi YY, Taniguchi M, Tsuge T, Oka A, Aoyama, T: Involvement of *Arabidopsis thaliana* Phospholipase Dζ2 in Root Hydrotropism through the Suppression of Root Gravitropism, *Planta*, **231,** 491-497 (2010).

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

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

Taniguchi M, Sasaki N, Tsuge T, Aoyama T, Oka A: ARR1 Directly Activates Cytokinin Response Genes that Encode Proteins with Diverse Regulatory Functions, *Plant Cell Physiol.*, **48,** 263-277 (2007).

Imai KK, Ohashi Y, Tsuge T, Yoshizumi T, Matsui M, Oka A, Aoyama T: The A-type Cyclin CYCA2;3 is a Key Regulator of Ploidy Levels in *Arabidopsis* Endoreduplication, *Plant Cell*, **18,** 382-396 (2006).

Mechanism Fixing and Sustaining the Polarity of Plant Cells

Root hairs have been used as a model system for studying molecular mechanisms involved in plant cell morphogenesis, because of their accessibility for experimental observation and a wide variety of their mutants. Root hairs are cellular protuberances resulting from the polar outgrowth of specific root epidermal cells called tricoblasts (Figure1). During root hair morphogenesis, a bulge is initially formed at the distal end on the outer tricoblast surface, the fixed position through a mechanism for planar polarity. Subsequently, the bulge protrudes further, perpendicular to the root surface, by highly polarized cell expansion, resulting in a thin cylindrical structure. This type of cell expansion is called tip growth, because all of the events involved in the growth, including cell wall and plasma membrane synthesis, are limited to the tip.

Figure 1. Root of *Arabidopsis thaliana*. A main root of a young seedling with root hairs is shown. Bar = 1 mm.

Once root hair tip growth begins, the polarity is strictly sustained, resulting in straight root hairs without branches. We hypothesized a mechanism for sustaining this highly polarized growth, which can not only localize events underlying cell expansion to the tip continuously but also maintain its own localization at the tip against the diffusion concomitant with cell expansion. This mechanism is possibly involved also in the planar polarity fixation, where regulatory factors for tip growth should be recruited to the locus of bulge initiation with a peaky pattern.

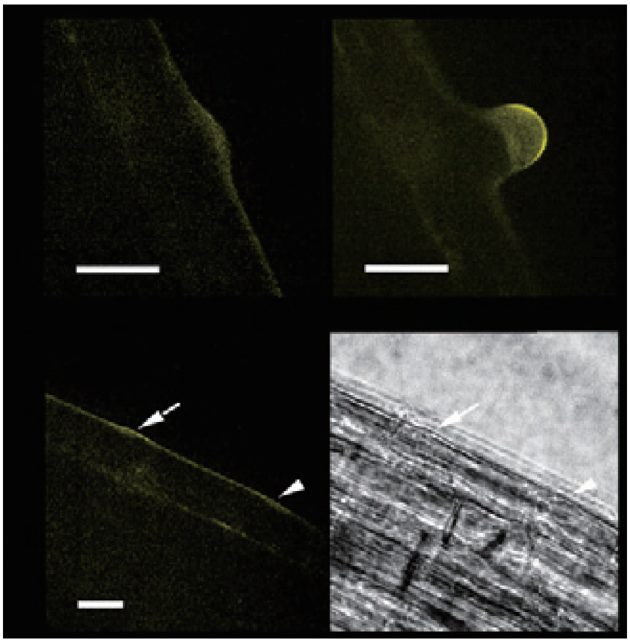


Figure 2. PIP5K3-YFP fusion protein driven by the *PIP5K3* promoter localized not only to apices of bulges (upper panels), but also to apparently flat sites where bulges were expected to appear (indicated by arrows in lower panels). Bar = 20 μm.

Of the regulatory factors identified so far for root hair tip growth in *Arabidopsis thaliana*, Rho-type GTPase of plants (ROP) and phosphatidylinositol 4-phosphate 5-kinase (PIP5K) are known to function positively. We found that PIP5K3 localizes to the bulge-expected position on the apical plasma membrane of tricoblasts similar to ROP2 (Figure 2). When both PIP5K3 and ROP2 were overexpressed in developing root hairs, synergistic effects on thier morphgenesis were observed; root hairs were abnormally elongated and branched (Figure 3). We assume that ROPs and phosphatidylinositol 4,5-bisphosphate produced by PIP5Ks are involved in the mechanism for sustaining the root hair tip growth.

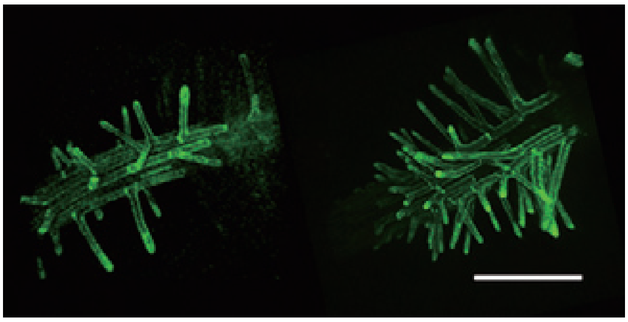


Figure 3. ROP2 overexpression caused slightly longer root hairs than normal (left panel). Additional overexpression of PIP5K3 resulted in even longer and branched root hairs (right panel). Bar = 20 μm.

Division of Biochemistry
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Proj Res**
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PD
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** PD (Res) (WPI) of Institute for Integrated Cell-Material Sciences
***Program-Specific Res (WPI) of Institute for Integrated Cell-Material Sciences
**** Institute for Integrated Cell-Material Sciences

Visitors

Assoc Prof CHANG, Young-Tae	National Univeristy of Singapore, Singapore, 14 May
Prof PARK, Hea-Young Choo	Ewha Womans University, Korea, R., 28 June–19 July
Assoc Prof DORE, Timothy	University of Georgia, USA, 2 July
Prof PIEL, Joern	University of Bonn, Germany, 2 September
Assoc Prof PARK, Seung Bum	Seoul National University, Korea, R., 7–9 October
Prof QUIOCHO, Florante A.	Baylor College of Medicine, USA, 29 November–10 December

Scope of Research

KEYWORDS
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

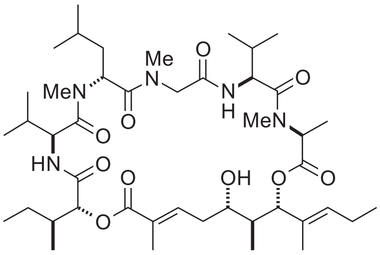
Chemical biology is often defined as "chemistry-initiated biology," in which scientists start with chemistry and end up understanding biology by utilizing chemical tools. Our laboratory has been discovering or designing small-molecule tools that modulate fundamental processes in human cells. Such small organic molecules often serve as tools for basic cell biology and/or for cell therapy. Discovery or design of small molecules with unique biological activity permits small-molecule initiated exploration of complex cellular events, and may also contribute to the realization of cell therapy. Although our primary goal is to provide chemical tools for biological investigations, we also hope to open new avenues for small-molecule applications in a range of fields.

Selected Publications

Shirakawa T, Kawazoe Y, Tsujikawa T, Jung D, Sato S, Uesugi M: Deactivation of STAT 6 through Serine 707 Phosphorylation by JNK, *J. Biol.Chem.*, (in press).
Sato S, Murata A, Orihara T, Shirakawa T, Suenaga K, Kigoshi H, Uesugi M: Marine Natural Product Aurilide Activates the OPA1-Mediated Apoptosis by Binding to Prohibitin, *Chem. Biol.*, (in press).
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 SREB, *Chem. Biol.*, **16 (8),** 882-892 (2009).
Yamazoe S, Shimogawa H, Sato S, Esko JD, 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: Wrenchnolol Derivative Optimized for Gene Activation in Cells, *J. Am. Chem. Soc.*, **131(13),** 4774-4782 (2009).

Mechanism of Action of Marine Natural Product Aurilide

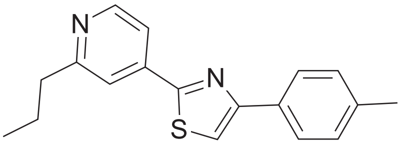
Aurilide is a potent cytotoxic marine natural product that induces apoptosis in cultured human cells at the pM to nM range; however, its mechanism of action has been unknown. Results of the present study showed that aurilide selectively binds to prohibitin 1 (PHB1) in the mitochondria, activating the proteolytic processing of optic atrophy 1 (OPA1), and resulting in mitochondria-induced apoptosis. The mechanism of aurilide cytotoxicity suggests that PHB1 is an apoptosis-regulating protein amenable to modulation by small molecules. Aurilide may serve as a small-molecule tool for studies of mitochondrion-induced apoptosis.



Aurilide

Fatostatin, A Small Molecule that Blocks Fat Synthesis

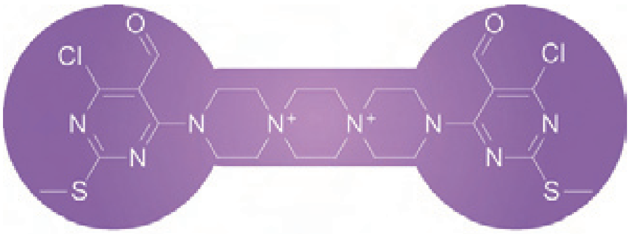
Sterol regulatory element binding proteins (SREBPs) are transcription factors that activate transcription of the genes involved in cholesterol and fatty acid biosynthesis. In the present study, we show that a small synthetic molecule we previously discovered to block adipogenesis is an inhibitor of the SREBP activation. The diarylthiazole derivative, now called fatostatin, impairs the activation process of SREBPs, thereby decreasing the transcription of lipogenic genes in cells. Our analysis suggests that fatostatin inhibits the ER-Golgi translocation of SREBPs through binding to their escort protein, the SREBP cleavage-activating protein (SCAP), at a distinct site from the sterol-binding domain. Fatostatin blocked increases in body weight, blood glucose, and hepatic fat accumulation in obese ob/ob mice, even under uncontrolled food intake. Fatostatin may serve as a tool for gaining further insights into the regulationof SREBP.



Fatostatin

Adhesamine, A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth

During an image-based phenotype screening of our chemical library, we noted a small molecule that boosts the adhesion and growth of human cells. Chemical and cell biological experiments suggest that the diaryldispiro-tripiperazine derivative (adhesamine) targets selective cell-surface glycosaminoglycans, especially heparan sulfate, for increasing cell adhesion and growth. The 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-Llysine, adhesamine induces apparently normal cell adhesion accompanied by organized actin structures and activation of focal adhesion kinase and ERK1/2 mitogen-activated protein kinases. Adhesamine may be useful as a cell-attaching reagent for cell engineering and basic cell biology.



Adhesamine

Wrenchnolol Derivative Optimized for Gene Activation in Cells

Naturally occurring transcription factors usually have two independent domains, a DNA-binding domain and an activation domain. In designing a synthetic small molecule that mimics a transcription factor,each of the two domains needs to be replaced by small-molecule counterparts. Results of the present study show that derivatives of wrenchnolol, a synthetic molecule that interacts with Sur-2 coactivator, serve as activation modules and stimulate gene transcription in vitro and in cells when tethered to a DNA-binding molecule. Thirteen derivatives of wrenchnolol were chemically synthesized and tested for their ability to activate transcription in vitro and in cells. When tethered to the GAL4 DNA-binding domain, one derivative increased transcription of a GAL4-responsive reporter gene in cells 9-fold. This optimized derivative also induced up to 45% myogenesis of C2C12 cells when tethered to the DNA-binding domain of myogenic transcription factor MyoD. This optimized derivative may serve as a starting point for designing biological tools or components of fully synthetic transcription factors that permit selective up-regulation of genes.

Division of Environmental Chemistry
– Molecular Materials Chemistry –

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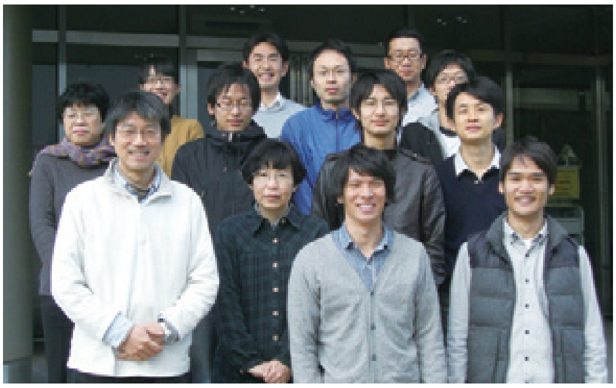
Mr ROTZOLL, Robert Georg-August-University of Göttingen, Germany, 4 November

Scope of Research

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

KEYWORDS

Solid-State NMR
Amorphous Materials
Organic Light-Emitting Diodes
Living Radical Polymerization
Quantum Chemical Calculation



Selected Publications

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

Goto A, Hirai N, Nagasawa K, Tsujii Y, Fukuda T, Kaji H: Phenols and Carbon Compounds as Efficient Organic Catalysts for Reversible Chain Transfer Catalyzed Living Radical Polymerization (RTCP), *Macromolecules*, **43,** 7971-7978 (2010).

Nishiyama Y, Fukushima T, Takami K, Kusaka Y, Yamazaki T, Kaji H: Characterization of Local Structures in Amorphous and Crystalline Tris(8-hydroxyquinoline) Aluminum(III) (Alq$_3$) by Solid-State ^{27}Al MQMAS NMR Spectroscopy, *Chemical Physics Letters*, **471,** 80-84 (2009).

Goto A, Zushi H, Hirai N, Wakada T, Tsujii Y, Fukuda T: Living Radical Polymerizations with Germanium, Tin, and Phosphorus Catalysts–Reversible Chain Transfer Catalyzed Polymerizations (RTCPs), *J. Am. Chem. Soc*., **129,** 13347-13354 (2007).

Kaji H, Kusaka Y, Onoyama G, Horii F: CP/MAS ^{13}C NMR Characterization of the Isomeric States and Intermolecular Packing in Tris(8-hydroxyquinoline) Aluminum(III) (Alq$_3$), *J. Am. Chem. Soc.*, **128,** 4292-4297 (2006).

Revealing Bipolar Charge-Transport Property of 4,4'-N,N'-dicarbazolylbiphenyl (CBP) by Quantum Chemical Calculations

4,4'-*N*,*N*'-dicarbazolylbiphenyl (CBP) has both the hole- and electron-transport ability, that is, bipolar charge-transport property, and has been widely used for organic light-emitting diodes (OLEDs). In this study, we explain the bipolar charge-transport property of CBP by quantum chemical calculations for the crystal. Both the reorganization energies and the charge transfer integrals were investigated, and charge-transfer rate constants were calculated based on Marcus theory. The hole- and electron-transfer rate constants thus calculated were found to be similar in magnitude. This is in sharp contrast with the case of a structurally similar but a poor electron-transport material, *N*,*N*'-diphenyl-*N*,*N*'-di(*m*-tolyl)benzidine (TPD), for which the hole-transfer rate constants were calculated to be much larger than the electron-transfer rate constants. From the detailed analysis of the charge transfer integrals for CBP, it was found that holes transfer through all the segments of the molecules, using the delocalized HOMO over the whole molecule as in the case of TPD. On the other hand, electrons transfer advantageously through the delocalized LUMO on the carbazole moieties of CBP, which have close intermolecular contacts. The LUMO of TPD localizes on the central biphenylene moiety, resulting in small electron transfer integrals. The results clearly show the difference of the electron-transport property between CBP and TPD.

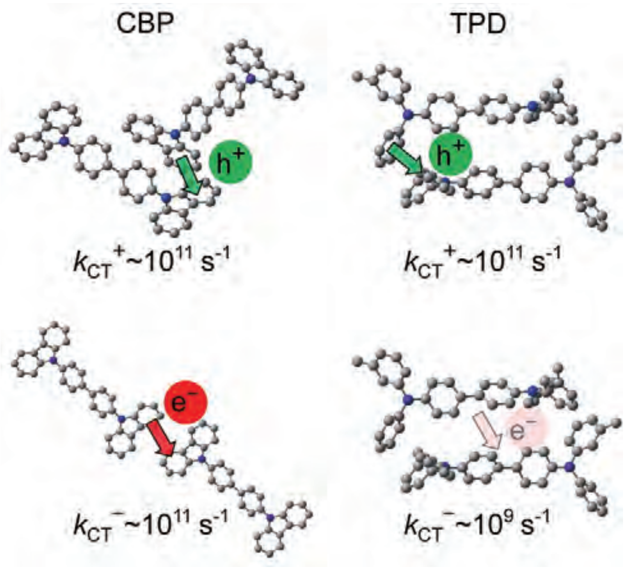
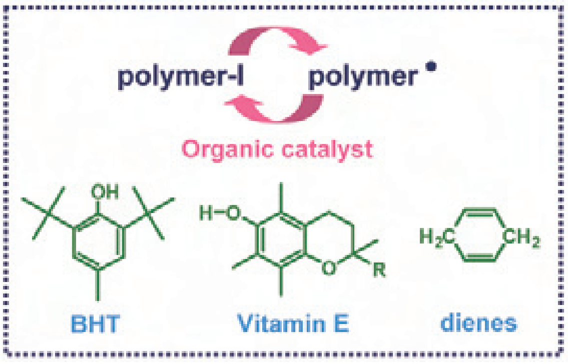


Figure 1. Structures of CBP and TPB and the charge transfer rate constants.

Phenols and Carbon Compounds as Efficient Organic Catalysts for Living Radical Polymerization

Simple phenols and hydrocarbons were successfully used as novel and efficient organic catalysts for reversible chain transfer catalyzed living radical polymerization (RTCP). This is the first use of oxygen- and carbon-centered compounds as catalysts of living radical polymerization. Low-polydispersity polystyrenes and polymethacrylates with predicted molecular weight were obtained with a fairly high conversion in a fairly short time. The catalysts include such common compounds as phenol itself, phenol-based antioxidants for foods and resins (e.g., 3,5-di-*t*-butyl-4-hydroxytoluene (BHT)), phenol-based natural antioxidants (e.g., vitamin E), and dienes (e.g., 1,4-cyclohexadiene). 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.



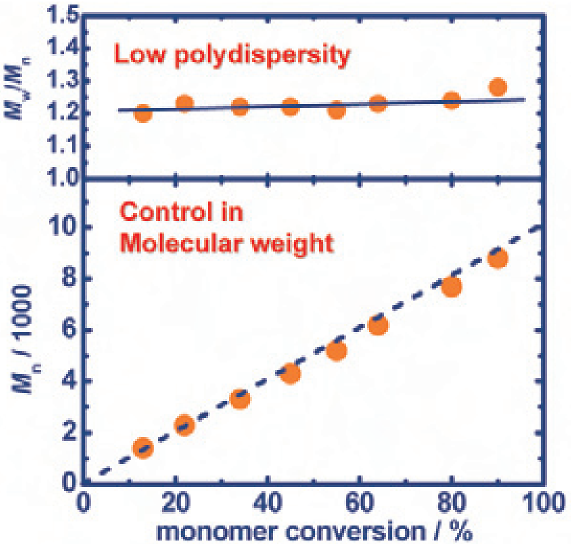


Figure 2. Plots of molecular weight (M_n) and molecular weight distribution (M_w/M_n) vs monomer conversion for a polymerization of methyl methacrylate with 1,4-cyclohexadiene (carbon-centered catalyst).

Division of Environmental Chemistry
– Hydrospheric Environment Analytical Chemistry –

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Dr BHUSHAN, Ravi	Physical Research Laboratory, India, 9 November

Scope of Research

(i) Biogeochemistry of trace elements in the hydrosphere: Novel analytical methods are developed for trace metals and isotopes. Distribution of trace elements in the hydrosphere and its effects on ecosystem are investigated. The study also covers hydrothermal activity, deep biosphere and paleocean.

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

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

[left] The last work day of Assist Prof Firdaus on 29 September 2010.
[right] Prof Yuan-Hui Li (University of Hawaii) and Lake Biwa on 26 April 2008.

Selected Publications

Li YH, Sohrin Y, Takamatsu T: Lake Biwa and the Ocean: Geochemical Similarity and Difference, *Limnology*, DOI: 10.1007/s10201-010-0326-0 (2010).

Minami T, Higo E, Nakatsuka S, Cid AP, Vu TDH, Norisuye K, Sohrin Y: Development of the Multielemental Determination Method for Bioactive Trace Metals in Open Ocean Seawater and Its Application to International Intercalibration, *Bunseki Kagaku*, **59,** 1087-1096 (2010) (in Japanese).

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 Research II*, **56,** 2822-2838 (2009).

Nakagawa Y, Firdaus ML, Norisuye K, Sohrin Y, Irisawa K, Hirata T: Precise Isotopic Analysis of Mo in Seawater Using Multiple Collector-Inductively Coupled Mass Spectrometry Coupled with a Chelating Resin Column Preconcentration Method, *Analytical Chemistry*, **80,** 9213-9219 (2008).

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

Lake Biwa and the Ocean: Geochemical Similarity and Difference

The average compositions of water, bottom sediments, Mn crusts and Mn concretions from Lake Biwa are re-examined, in conjunction with those of seawater, oceanic pelagic clay, and deep-sea Mn nodules. The purpose is to gain additional insights into the geochemical behaviors of elements in Lake Biwa and the ocean, which are quite different in ionic strength, pH, water residence times, sediment accumulation rates, carbon fluxes to sediments, and the redox potential in sediments. Excluding a few millimeters of oxic surface sediment, there is no appreciable accumulation of Mn in the Lake Biwa bottom sediments, due to reducing condition there. Consequently, other B-type cations (such as Fe, Ga, Cu, Pb, Co, Sn, and Bi; with sub-shell valence electron configuration of d1-10) are also less concentrated in the lake sediments than in the oceanic pelagic clay. In turn, B-type cations have much higher dissolved concentrations in the lake water than in the ocean. Rare earth elements (REE) mainly form organic complexes in the lake water, and carbonate complexes in the ocean (Figure 1). REE are mostly associated with detritus aluminosilicate phases in the Lake Biwa sediments, but with phosphate phases in the deep sea sediments. Fe and Mn oxide phases are clearly separated in marine Mn nodules and crusts, but not in Mn crusts and concretions from Lake Biwa. Useful parameters such as the enrichment factor and the distribution coefficient of elements between solid and liquid phases were estimated in both systems for further discussions.

This study was done in cooperation with Prof Yuan-Hui Li (University of Hawaii) and Prof Takejiro Takamatsu (Ibaraki University).

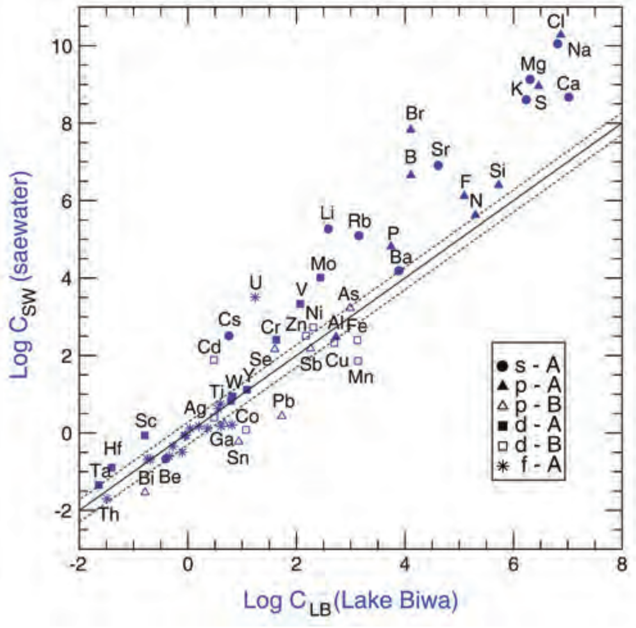

Figure 1. The average concentrations of elements (10^{-9} g/L) in Lake Biwa water (C_{LB}) versus that in seawater (C_{SW}). All in logarithm scale.

Ion Imprinted Sol-gel Materials for the Separation of Metal Ions

Much attention has been paid to a molecular (ion) imprinting technique as a method to prepare highly selective adsorbents. Recently, a novel organic-inorganic hybrid sorbent was proposed by Dai et al. employing Cu(II) and surfactant micelles as templates. We prepared some new sorbents based on this hierarchical double-imprinting concept using Cu(II), Zn(II), Ni(II), Co(II), Cd(II) and Pd(II) as templates (Figure 2).

The sorbents were prepared through self-hydrolysis, self-condensation, and co-condensation of the cross-linking agent (tetraethylorthosilicate) and the functional precursor in an alkaline media in the presence of cetyltrimethylammonium bromide. The bifunctional ligands such as 3-(2-aminoethylamino)propyltrimethoxysilane (AAPTS) and 3-(2-aminoethylamino)methyltrimethoxysilane (AAMTS) were employed.

Adsorption of Cu(II) and Zn(II) to Cu imprinted sorbent with AAMTS (Cu/AAMTS) and to control blank sorbent (non/AAMTS) has been examined. 23% of Cu(II) and 20% of Zn(II) were adsorbed to non/AAMTS sorbent, and 99% and 22% to Cu/AAMTS. The effect of Cu(II) imprinting is quite meaningful for AAMTS rather than AAPTS. The adsorptions of metal ions to Zn(II), Ni(II), Co(II), Cd(II) and Pd(II) imprinted sorbents were also examined.

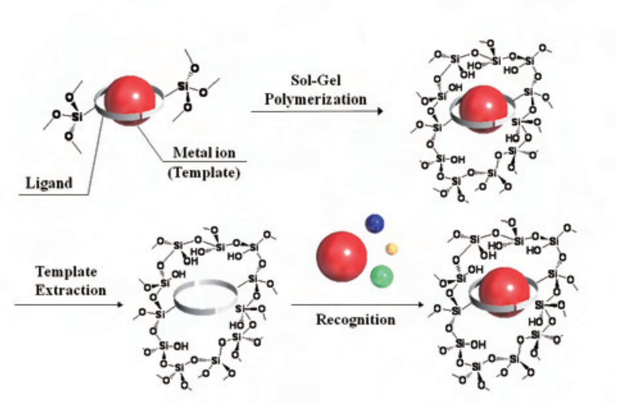

Figure 2. Ion imprinted functional silica gel sorbent.

Division of Environmental Chemistry
– Solution and Interface Chemistry –

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Mr MARSALEK, Ondrej	Czech Academy of Science, Czech Republic, 25 January–31 March
Dr FEDOROV, Maxim V	Max Planck Institute, Germany, 12–14 March

Scope of Research

The structure, dynamics, and reaction of solutions with nano-scale inhomogeneity and/or with fine tunability are investigated by NMR spectroscopy, computer simulation, and statistical-mechanical theory of solutions, 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.

KEYWORDS

Lipid Membrane
Supercritical Fluid
Ionic Liquid
Free Energy
Dynamic Inhomogeneity

Selected Publications

Yasaka Y, Wakai C, Matubayasi N, Nakahara M: Rotational Dynamics of Water and Benzene Controlled by Anion Field in Ionic Liquids: 1-butyl-3-methylimidazolium Chloride and Hexafluorophosphate, *J. Chem. Phys*, **127,** 104506 (8 pages) (2007).

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

Takahashi H, Ohno H, Kishi R, Nakano M, Matubayasi N: Computation of the Free Energy Change Associated with One-electron Reduction of Coenzyme Immersed in Water: A Novel Approach within the Framework of the Quantum Mechanical/molecular Mechanical Method Combined with the Theory of Energy Representation, *J. Chem. Phys.*, **129,** 205103 (14 pages) (2008).

Yoshida K, Matubayasi N, Uosaki Y, Nakahara M: Scaled Polynomial Expression for Self-Diffusion Coefficients for Water, Benzene, and Cyclohexane over a Wide Range of Temperatures and Densities, *J. Chem. Eng. Data*, **55,** 2815–2823 (2010).

Karino Y, Fedorov MV, Matubayasi N: End-point Calculation of Solvation Free Energy of Amino-acid Analogs by Molecular Theories of Solution, *Chem. Phys. Lett.*, **496,** 351–355 (2010).

Dynamical Inhomogeneity of Lipid Membrane

The dynamical inhomogeneity in the lipid membrane is studied over a wide range of curvature by the solution-state ^{1}H NMR-nuclear Overhauser effect (NOE). To make possible the NOE measurement for large vesicles, the transient NOE method is combined with the spin-echo method (transient NOE-SE method) and is applied to micelle of 1-palmitoyl-lysophosphatidylcholine (PaLPC) with a diameter of 5 nm and to vesicles of dipalmitoylphosphatidylcholine (DPPC) with diameters ranging from 30 to 800 nm. The transient NOE-SE method suppresses the broad components in model-membrane signals and enables quantitative assessment of the NOE intensities even for an almost flat bilayer of ~800 nm in diameter. It is found that the NOE intensity increases with the diameter up to ~100 nm, and the model membrane is considered flat beyond ~100 nm. While the NOE between the hydrophilic choline and hydrophobic terminal methyl groups is absent for micelle as expected, its intensity is comparable to that for the neighboring group for vesicles of larger diameters. The origin of NOE signals between distant sites is revealed by MD analysis. The MD simulation is performed for the PaLPC micelle and the DPPC flat bilayer, and the time correlation function determining the NOE cross intensity is calculated. The corresponding correlation time for the DPPC flat bilayer enhances to microsecond and is shown to yield an observable NOE signal even for the hydrophilic terminal and hydrophobic terminal sites. Since the correlation time depends on the proton pairs by orders of magnitude, the NOE intensity for large vesicle is combined information of distance and dynamics and does not reflect only the distance. The correlation time in large vesicle is then determined by employing the experimental NOE intensity and the MD-based distance distribution. It is found to vary by three orders of magnitude over the proton sites in the case of large vesicles.

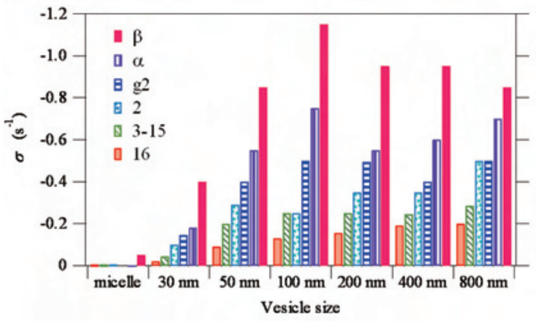

Figure 1. The vesicle size dependence of the cross relaxation rate constant σ between the γ site and the other sites at 60ºC.

Free-Energy Analysis of Hydration Effect on Protein with Explicit Solvent

Hydration is a key factor for controlling the stability and fluctuation of protein structure. In the statistical thermodynamic context, the hydration effect is quantified by the solvation free energy and is affected by specific protein-water intermolecular interactions. In the present work, the relationship between the protein conformation and the hydration effect is investigated for the equilibrium fluctuation of cytochrome *c*. To elucidate the hydration effect with explicit solvent, the solvation free energy of the protein immersed in water was calculated using the molecular dynamics simulation coupled with the method of energy representation. As shown in Figure 2, the protein intramolecular energy and the solvation free energy are found to compensate each other in the course of equilibrium fluctuation. The energy variation corresponding in magnitude to the formation/breakage of several tens of hydrogen bonds is induced and compensated by the solvent water. The correlation of the solvation free energy is further examined against the average sum of protein-water interaction and the excluded-volume part of the solvation free energy. The average sum is dominated by the electrostatic interaction and varies in proportion to the solvation free energy. The excluded-volume part has no correlation to the (total) solvation free energy and is virtually constant. The variation of the solvation free energy in response to the conformational fluctuation at equilibrium is described by the linear-response-type relationship with the protein-water interaction supplemented by an offset representing the excluded-volume effect.

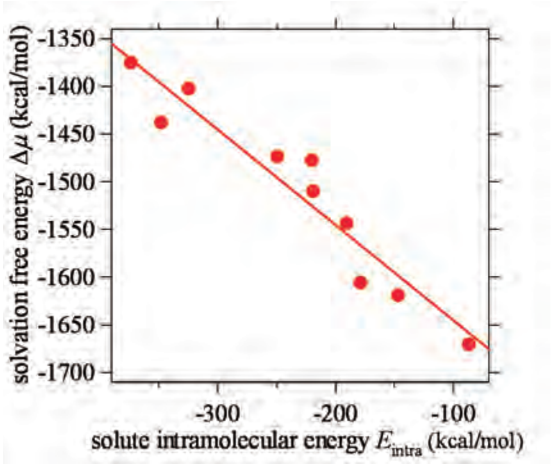

Figure 2. The solvation free energy $\Delta\mu$ of cytochrome *c* plotted against the intramolecular energy E_{intra}. The solid line represents the least-square fit and is given by $E_{\text{intra}} + \Delta\mu = -1.7\times10^3$ kcal/mol.

Division of Environmental Chemistry
– Molecular Microbial Science –

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WANG, Yu (M2)
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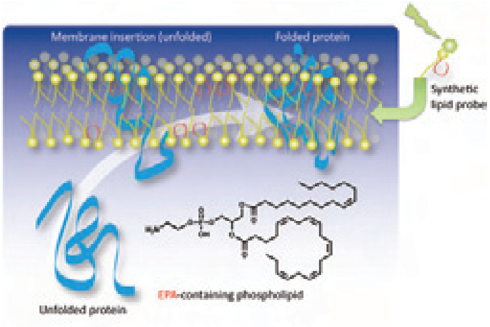
FUJIMOTO, Naofumi (M1)
TARUI, Jun (M1)

Visitors

Prof KROL, Alain	Centre National de la Recherche Scientifique (CNRS), France, 9 February
Prof ARNER, Elias	Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Sweden, 8 June

Scope of Research

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



KEYWORDS

Molecular Microbial Science
Biochemistry
Psychrotroph
Polyunsaturated Fatty Acids
Bioengineering

Selected Publications

Zhang W, Urban A, Mihara H, Leimkuhler S, Kurihara T, Esaki N: IscS Functions as a Primary Sulfur-donating Enzyme by Interacting Specifically with MoeB and MoaD in the Biosynthesis of Molybdopterin in *Escherichia coli*, *J Biol Chem*, **285,** 2302-2308 (2010).

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Mowafy AM, Kurihara T, Kurata A, Uemura T, Esaki N: 2-Haloacrylate Hydratase, a New Class of Flavoenzyme that Catalyzes the Addition of Water to the Substrate for Dehalogenation, *Appl Environ Microbiol*, **76,** 6032-6037 (2010).

Kawamoto J, Kurihara T, Yamamoto K, Nagayasu M, Tani Y, Mihara H, Hosokawa M, Baba T, Sato SB, Esaki N: Eicosapentaenoic Acid Plays a Beneficial Role in Membrane Organization and Cell Division of a Cold-adapted Bacterium, *Shewanella livingstonensis* Ac10, *J. Bacteriol.*, **191,** 632-640 (2009).

Studies on Dynamics of Eicosapentaenoic-acid-containing Phospholipids by Using Fluorescence-labeled Ether Phospholipids

Shewanella livingstonensis Ac10, a psychrotrophic Gram-negative bacterium isolated from Antarctic seawater, grows at a temperature range from 4˚C to 25˚C. This bacterium produces eicosapentaenoic acid (EPA), a long-chain polyunsaturated fatty acid, as an acyl component of membrane phospholipids at low temperatures close to 0˚C. We identified the genes required for synthesis of EPA and disrupted them to obtain EPA-less mutants. The mutants lacking EPA showed significant growth retardation at 4°C but not at 18°C. Supplementation of a synthetic phosphatidylethanolamine containing EPA at the *sn*-2 position complemented the growth defect. The EPA-less mutant became filamentous, and multiple nucleoids were observed in a single cell at 4°C, indicating that the mutant has a defect in cell division.

To analyze the physiological function of EPA, we synthesized fluorescence-labeled phospholipids shown in Figure 1 as molecular probes to visualize the localization of EPA-containing phospholipids. In AcylalkylEPA and DialkylEPA, the eicosapentaenyl group is bound to the glycerol backbone of the phospholipid by an ether bond to prevent separation of EPA and the fluorescence group by hydrolysis *in vivo*. These fluorescent phospholipids were added to the EPA-less mutant of *S. livingstonensis* Ac10, and the cells were grown at 4–7˚C for fluorescence microscopic analysis. When AcylalkylEPA was used, fluorescence was localized between two nucleoids at the center of the cells during cell division, suggesting that EPA-containing phospholipids are involved in this cellular process (Figure 2).

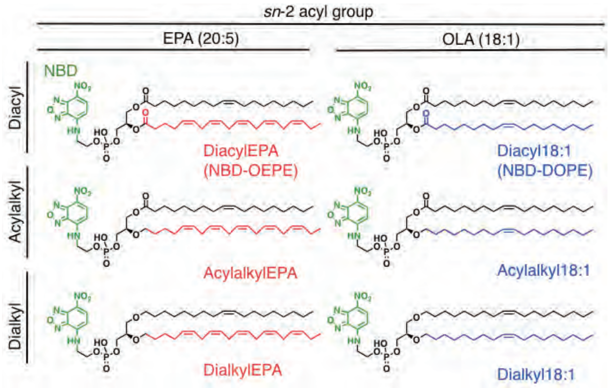

Figure 1. Fluorescent phospholipids synthesized in this study to analyze the physiological role of EPA.

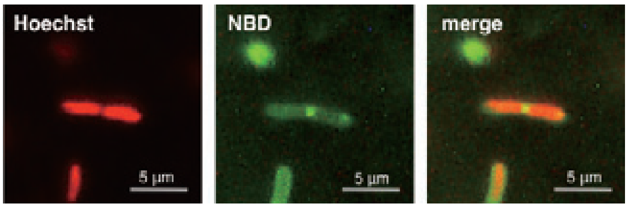

Figure 2. Fluorescence microscopic images of an EPA-less mutant cell that incorporated AcylalkylEPA. Nucleoids were stained with Hoechst.

Physiological Role of Eicosapentaenoic-acid-containing Phospholipids in the Folding of a Cold-inducible Membrane Protein of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10

Polyunsaturated fatty acids (PUFA), such as eicosapentaenoic acid (EPA) and docosahexaenoic acid, are known to have various beneficial effects on human health. PUFAs existing as acyl components of membrane phospholipids alter the physicochemical properties of lipid bilayers, including permeability, curvature, fluidity, and thickness, and affect the function of membrane proteins. However, molecular mechanisms how PUFAs influence the functions of membrane proteins are not well understood. A cold-adapted microorganism, *Shewanella livingstonensis* Ac10 isolated from Antarctic seawater, produces EPA as an acyl chain of its membrane phospholipids at 4˚C. In order to elucidate the physiological role of EPA at low temperatures, we performed *in vitro* reconstitution of a cold-inducible membrane protein, OmpC74, with the liposomes containing or not containing EPA and analyzed the effect of the presence of EPA on the folding of OmpC74. The larger amounts of folded OmpC74 were observed in the liposomes containing EPA than those without EPA. Circular dichroism analysis indicated that OmpC74 rapidly interacts with the membrane surface and forms ß-sheet structures in the EPA-containing liposome at 4˚C. These results suggest that EPA-containing phospholipids play a role as a molecular chaperone in the membrane insertion and folding of OmpC74 at low temperatures.

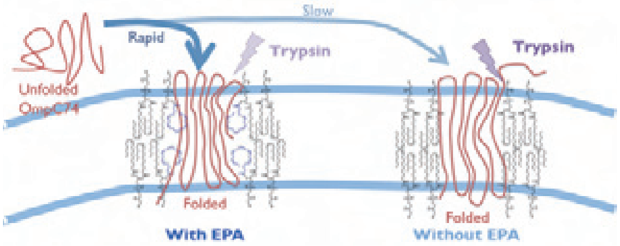

Figure 3. EPA-containing phospholipids accelerate the membrane insertion and folding of a cold-inducible outer membrane protein, OmpC74, at low temperatures.

Division of Multidisciplinary Chemistry
– Polymer Materials Science –

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HARA, Ayana (UG)
JIN, Ling (RS)

Visitor

Prof GABRYS, Barbara J University of Oxford, UK, 21 May

Scope of Research

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

KEYWORDS
Polymer Physics
Polymer Properties
Scattering
Neutron Scattering

Selected Publications

Kanaya T, Inoue R, Kawashima K, Miyazaki T, Tsukushi I, Shibata K, Matsuba G, Nishida K, Hino M: Glassy Dynamics and Heterogeneity of Polymer Thin Films, *J. Phys. Soc. Jpn.*, **78,** [041004-1]-[041004-9] (2009).

Ogawa H, Kanaya T, Nishida K, Matsuba G, Majewski JP, Watkins E: Time-resolved Specular and Off-specular Neutron Reflectivity Measurements on Deuterated Polystyrene and Poly(vinyl methyl ether) Blend Thin Films during Dewetting Process, *J. Chem. Phys.*, **131,** [114907-1]- [114907-7] (2009).

Rahman N, Kawai T, Mastuba G, Nishida K, Kanaya T, Watanabe H, Okamoto H, Kato M, Usuki A, Matsuda M, Nakajima K, Honmma N: Effect of Polylactide Stereocomplex on the Crystallization Behavior of Poly(L –lactic acid), *Macromolecules*, **42,** 4739-4745 (2009).

Nishida K, Ogawa H, Matsuba G, Konishi T, Kanaya T: A High-resolution Small-angle Light Scattering Instrument for Soft Matter Studies, *J. Appl. Cryst.*, **41,** 732-728 (2008).

In-situ Observation of Crystallization of Isotactic Polypropylene from Mesomorphic Phase

We have studied crystallization behaviour of isotactic polypropylene (iPP) from mesomorphic phase in structural point of view. Time-resolved wide-angle X-ray diffraction (WAXD) measurements during a heating process have been performed using a synchrotron radiation (SR) X-ray beam line at SPring-8, Japan. The heating process was so programmed to reproduce a thermal trace of differential scanning calorimetry (DSC) with a constant heating rate (10 °C/min) in order to compare the structural change with thermal behaviour. SR-WAXD sensitively detected the crystallization behaviour (Figure 1) and we have obtained fractions of alpha-crystal, mesomorphic and amorphous phases as a function of temperature. During the crystallization, not the amorphous fraction but the mesomorphic one is mainly consumed (meso-alpha transition). We have also determined the energy level of the mesomorphic phase (meta-stable state) relative to that of alpha-crystal (stable state), considering the balance among the fractions of alpha-crystal, mesomorphic and amorphous phases.

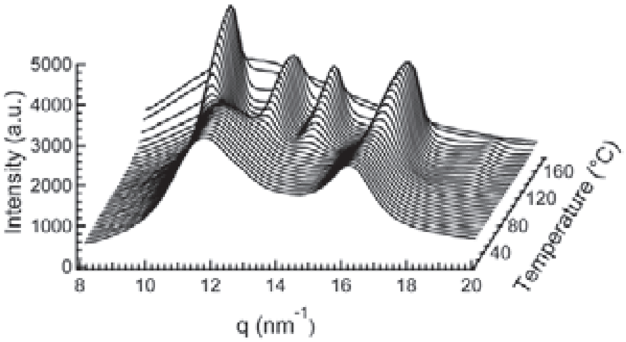

Figure 1. WAXD profiles during heating process from 30 to 170 °C displayed at every 5 °C from bottom to top. The profiles were shifted diagonally for clarification.

Dynamics of Amorphous Polymer Studied by Muon

The mechanism of glass transition and related glassy dynamics of glass-forming materials are still unresolved although so many experimental approaches have been conducted in the last two decades. To offer the new insight on the unresolved problems of dynamics of amorphous materials, we have studied the dynamics of amorphous polybutadiene (PB) by muon spin resonance (μSR). We have performed longitudinal field (LF) measurements with a 100 G magnetic field at temperatures from 10 K to 300 K. Figure 2 (a) shows an example of the decay of asymmetry for PB at 300 K and we could observe a decay of asymmetry originated from the dynamics of PB. The temperature dependence of relaxation rate is shown in Figure 2 (b) and the relaxation rate increased monotonically with temperature up to 180 K. Above 180 K (which is near to glass transition temperature of PB), we could observe a steep increase of relaxation rate, implying that the glass transition was detected by μSR. In addition to the detection of glass transition, we also observed a small increase of relaxation rate at round 120 K. This temperature corresponded to the onset temperature of local motion with the time scale of ps. From μSR studies, we succeeded to detect the dynamics of PB on a wide-time scale.

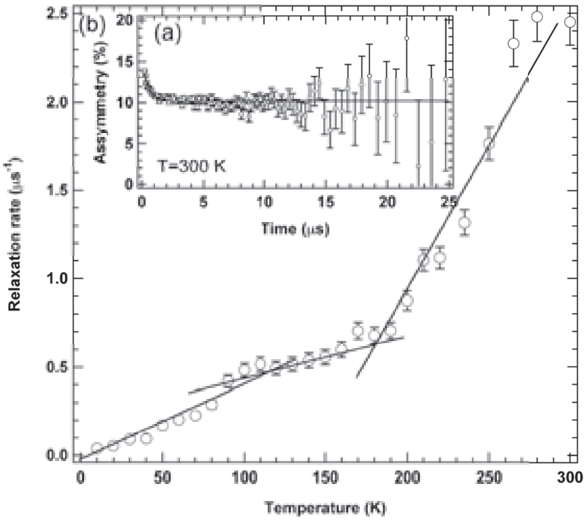

Figure 2. (a) Time dependence of the decay of asymmetry for PB at 300 K under a LF of 100 G. (b) Temperature dependence of the decay rate for PB. Lines are shown to clearly observe the onset of relaxation.

Division of Multidisciplinary Chemistry
– Molecular Rheology –

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


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KAWASAKI, Yohji (M1)
KITANO, Jun-ya (M1)
YAMAMOTO, Satoshi (UG)
TACHIIRI, Akihiro (UG)

Visitors

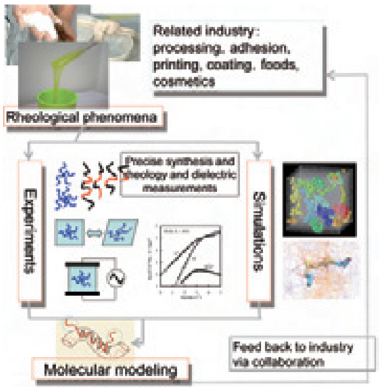
Prof MCLEISH, Tom	Durham University, UK, 11–12 August
Prof KEUNINGS, Roland	Université Catholique de Louvain, Belgium, 15–17 August
Prof AHN, Kyung Hyun	Seoul National University, Korea, R., 8–9 August
Prof SUN, Kang	Shanghai Jiao Tong University, China, P.R., 8–10 August
Prof KWON, Youngdon	Sungkyunkwan University, Korea, R., 8–10 August
Prof YU, Wei	Shanghai Jiao Tong University, China, P.R., 8–10 August
Prof SHAQFEH, Eric	Stanford University, USA, 8–10 August
Prof CHO, Kwang Soo	Kyungpook National University, Korea, R., 8–10 August
Dr TAO, Ke	Shanghai Jiao Tong University, China, P.R., 20 March – 20 June, 8–10 August
Prof SHEN, Amy	University of Washington, USA, 8–10 August
Prof FRIED, Eliot	McGill University, Canada, 8–10 August
Prof DUDA, Fernando	Federal University of Rio de Janeiro, Brazil, 8–10 August

KEYWORDS

Rheology
Softmatters
Polymers
Emulsions
Suspensions

Scope of Research

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



Selected Publications

Uno A, Matsumiya Y, Masubuchi Y, Watanabe H: Rheological and Dielectric Behavior of Polyisoprene under Pressurized Carbon Dioxide, *J. Soc. Rheol. Jpn.*, **38(3),** 117-123 (2010).

Furuichi K, Nonomura C, Masubuchi Y, Watanabe H: Chain Contraction and Nonlinear Stress Damping in Primitive Chain Network Simulations, *J. Chem. Phys.*, **133,** [174902-1]-[174902-10] (2010).

Chen Q, Uno A, Matsumiya Y, Watanabe H: Viscoelastic Mode Distribution of Moderately Entangled Linear Polymers, *J. Soc. Rheol. Jpn.*, **38(5),** 187-193 (2010).

Rheological and Dielectric Behavior of Polyisoprene under Pressurized Carbon Dioxide

For a well-entangled polyisoprene (PI; molecular weight = 260k) equilibrated under pressurized carbon dioxide (CO_2) at 25 °C, linear viscoelastic and dielectric data, respectively, were measured with a stress-controlled rheometer and a dielectric bridge being equipped with respective high-pressure cells. The viscoelastic and dielectric data shifted to higher frequencies with increasing CO_2 pressure, indicating that the pressurized CO_2 dissolved into PI thereby accelerating the global motion of PI. For those data at various CO_2 pressure, time-CO_2 pressure superposition held well and a single master curve was obtained, and the horizontal/vertical shift factors were consistent for the viscoelastic and dielectric data. These results indicated that the dissolved CO_2 behaved just as an ordinal solvent to accelerate the global motion of PI as in ordinary solutions. In fact, the dynamic tube dilation (DTD) relationship between the viscoelastic and dielectric data, known to be valid for ordinary solutions/bulk of linear PI, was found to work also the PI/CO_2 system, which confirmed the simple solvent role of the pressurized CO_2 for the global motion of PI. Thus, the knowledge for ordinary polymer solutions would work for processing of polymer/CO_2 systems.

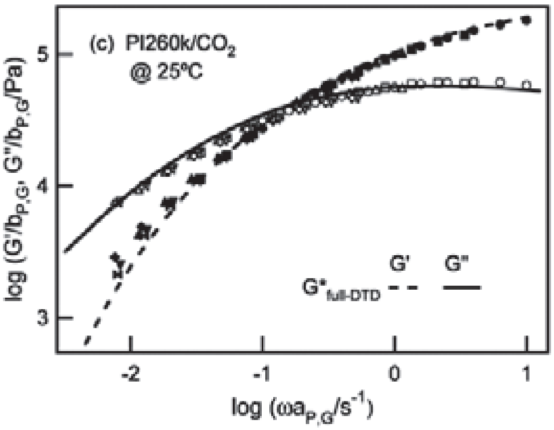


Figure 1. Linear viscoelastic storage and loss moduli measured for PI260k equilibrated under various pressures of CO_2 at 25 °C after time-CO_2 pressure superposition. Dashed and solid curves show *G'* and *G''* calculated from the dielectric data through the full-DTD relationship.

Chain Contraction and Nonlinear Stress Damping in Primitive Chain Network Simulations

Doi and Edwards (DE) proposed that the relaxation of entangled linear polymers under large deformation occurs in decoupled two steps: the fast chain contraction (via the longitudinal Rouse mode of the chain backbone) and the slow orientational relaxation (due to reptation). However, this decoupling is invalid for a generalized convective constraint release (CCR) mechanism that releases the entanglement on every occasion of the contraction of surrounding chains. Thus, we conducted primitive chain network simulations to investigate the chain contraction under step shear. The simulation quantitatively reproduced experimental features of the nonlinear relaxation modulus $G(t,\gamma)$. Namely, $G(t,\gamma)$ was cast in the time-strain separable form, $G(t,\gamma)=h(\gamma)G(t)$ with $h(\gamma)$=damping function and $G(t)$=linear modulus, but this rigorous separability was valid only at times t comparable to the terminal relaxation time, although a deviation from this form was rather small (within 10%) at $t > \tau_R$ (longest Rouse relaxation time). A molecular origin of this delicate failure of time-strain separability at $t \sim \tau_R$ was examined for the chain contour length. The contributions of the terminal reptative mode to the chain length relaxation emerged because the sliplinks (entanglement) were removed via the generalized CCR mechanism and the reformation of the sliplinks was slow at around the chain center. The number of monomers in the subchain was kept larger at the chain center than at the chain end, thereby reducing the tension at the chain center compared to the DE prediction. This reduction of the tension prevented completion of the length equilibration at $t \sim \tau_R$ and it forced the equilibration to complete through the reptative mode. The delicate failure of time-strain separability seen for $G(t,\gamma)$ at $t \sim \tau_R$ reflects this retarded length equilibration.

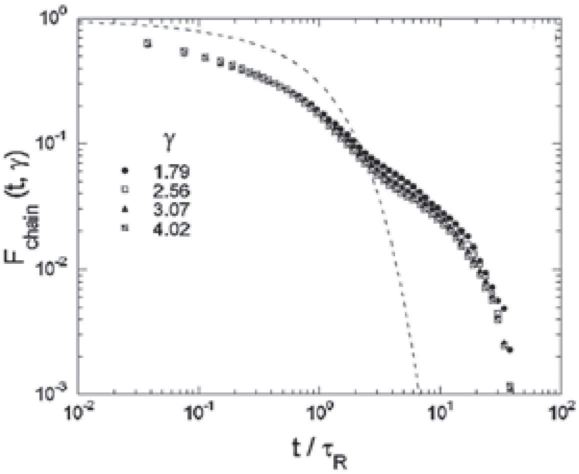


Figure 2. Relaxation of contour length of the chain after various step shear deformations with strain at γ. Dashed lines indicate the prediction of DE theory.

Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

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

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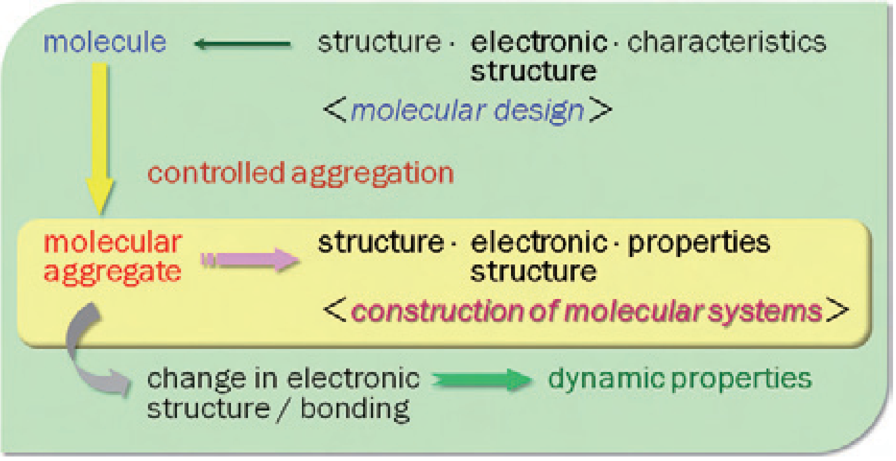
YOSHINAGA, Kengo (M2)	YASUNISHI, Koji (M1)

Scope of Research

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

KEYWORDS

Dielectric Spectroscopy
Erythrocyte
Surface Potential
Thin Film
Zwitterionic Molecule



Selected Publications

Hayashi Y, Katsumoto Y, Oshige I, Omori S, Yasuda A, Asami K: Dielectric Inspection of Erythrocytes, *J. Non-Cryst. Solids*, **356,** 757-762 (2010).

Tsutsumi J, Yoshida H, Murdey R, Sato N: Spontaneous Buildup of Surface Potential with a Thin Film of a Zwitterionic Molecule Giving Non-Centrosymmetric Crystal Structure, *Appl. Phys. Lett.*, **95,** 182901 (2009).

Murdey R, Bouvet M, Sumimoto M, Sakaki S, Sato N: Direct Observation of the Energy Gap in Lutetium Bisphthalocyanine Thin Films, *Synth. Met.*, **159,** 1677-1681 (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).

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

Yoshida H, Inaba K, Sato N: X-ray Diffraction Reciprocal Space Mapping Study of the Thin Film Phase of Pentacene, *Appl. Phys. Lett.*, **90,** 181930 (2007).

Spontaneous Buildup of Surface Potential with a Thin Film of a Zwitterionic Molecule Giving Noncentrosymmetric Crystal Structure

Surface potentials were examined using the Kelvin method for thin films of zwitterionic molecules, pyridinium 1,3-dihydro-1,3-dioxo-2*H*-inden-2-ylide (PI) or 2-*N*-pyridinium-1,3-indandione betaine (IPB) and its nitrogen substituted compounds: pyridinium 5,7-dihydro-5,7-dioxo-6*H*-cyclopenta[*b*]pyridin-6-ylide (4N-PI) and pyridinium 5,7-dihydro-5,7-dioxo-6*H*-cyclopenta[*c*]pyridin-6-ylide (5N-PI), as well as pentacene as a control material. Among the three zwitterionic compounds, we recently confirmed that only 4N-PI molecules crystallize in a noncentrosymmetric structure with a space group *Pc* where all the molecular dipole moments point in the same direction. Spontaneous buildup of the surface potential on the film 5.5 V at a film thickness of 300 nm was observed only for 4N-PI (Figure 1). The relationship between the alignment of the molecular dipole moments in the film and the measured surface potentials was investigated using grazing incidence x-ray diffraction (GIXD), pole-figure measurements, atomic force microscopy (AFM), and Kelvin probe force microscopy (KFM). These structural analyses disclosed that the 4N-PI film contains small crystallites with the noncentrosymmetric crystallographic structure which is the same as its single crystal. Further, the crystallites are oriented with the (110) axes perpendicular to the substrate surface with a broad distribution width of about 20° (Figure 2). This result indicates that polar molecules crystallizing in the noncentrosymmetric structure can also show spontaneous surface potential when a preferred film structure is realized.

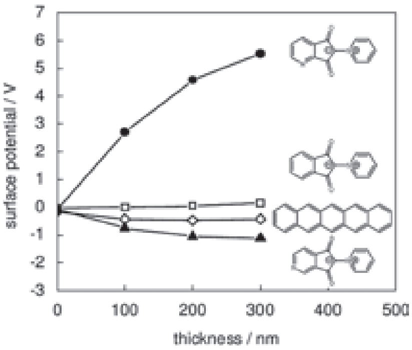


Figure 1. Surface potential measured for the films in the dark as a function of film thickness.

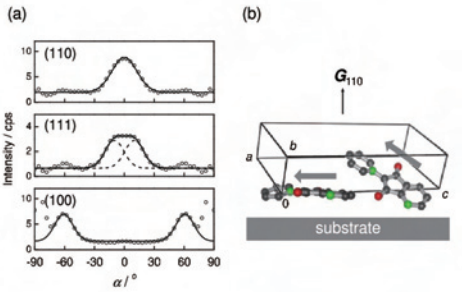


Figure 2. (a) X-ray pole figures (plotted as a function of polar angle *α* measured from the surface normal) of (110), (111) and (100) diffractions for the 4N-PI film. (b) Schematic of the analyzed orientation of the unit cell with 4N-PI molecules on the substrate surface.

Dielectric Spectroscopy Reveals Nanoholes of Erythrocyte Membrane Ghosts

When blood is diluted with water, erythrocytes swell and then burst to release hemoglobin molecules. The remaining membranes, called “ghosts”, are resealed under physiological conditions. About 50 years ago, Schwan and Carstensen reported that ghost suspensions showed peculiar dielectric dispersion below 10 kHz, called α-dispersion, which was not found for intact erythrocyte suspensions. The findings, however, have never been traced because of difficulty in low-frequency measurement due to electrode polarization, and therefore the origin of the α-dispersion has not been understood. This study has disclosed the α-dispersion (see Figure 3) by solving the problem in measurement using a new electrode configuration. The α-dispersion was found to be quite unstable at room temperature, being stabilized by fixation of ghosts with glutaraldehyde. The properties of the α-dispersion were exactly interpreted by the existence of a hole in each ghost membrane. The numerical simulation with a spherical cell model with a hole provided a linear relation between the characteristic frequency f_α of the α-dispersion and the hole radius R_h, and thereby the values of R_h being determined from those of f_α straightforwardly. The estimated values of R_h were close to those obtained by electron microscopy and several times larger than those from the analysis of the diffusion of probe molecules through the holes.

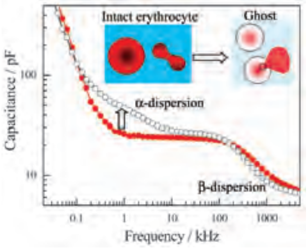


Figure 3. The capacitance of intact erythrocyte (closed circle) and ghost (open circle) suspensions plotted against the frequency of the applied ac field.

Division of Multidisciplinary Chemistry
– Supramolecular Biology –

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PD
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Res Associate (pt)

YAMAGUCHI, Yukiko

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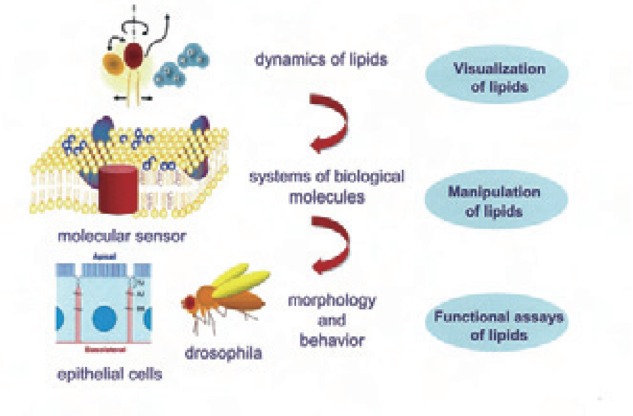
YAMAMOTO, Masatoshi (M2)
TANABE, Aiko (M2)
SUZUKI, Mayu (M1)

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.



KEYWORDS

Lipid Cell Biology Membrane

Selected Publications

Ikenouchi J, Umeda M: FRMD4A Regulates Epithelial Polarity by Connecting Arf6 Activation with the PAR Complex, *Proc. Natl. Acad. SCi. USA*, **107,** 748-753 (2010).

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).

Ikenouchi J, Sasaki H, Tsukita S, Furuse M, Tsukita S: Loss of Occludin Affects Tricellular Localization of Tricellulin, *Mol. Biol. Cell.*, **19(11),** 4687-4693 (2008).

Ikenouchi J, Umeda K, Tsukita S, Furuse M, Tsukita S: Requirement of ZO-1 for the Formation of Belt-like Adherens Junctions during Epithelial Cell Polarization, *J. Cell Biol.*, **176,** 779-786 (2007).

Emoto K, Inadome H, Kanaho Y, Narumiya S, Umeda M: Local Change in Phospholipid Composition at the Cleavage Furrow is Essential for Completion of Cytokinesis, *J. Biol. Chem.*, **280,** 37901-37907 (2005).

Regulation of Membrane Phospholipid Dynamics and Its Role in Cell Migration

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

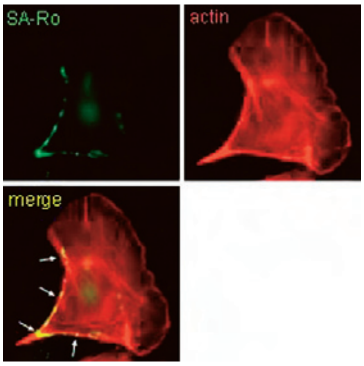


Figure 1. Cell-surface PE distributes in the inner leaflet of the ruffling membranes in migrating cells. The serum-stimulated cells were incubated with 10 μg/ml PE-binding peptide (SA-Ro) for 30 min at 37 °C, and then fixed and stained for SA-Ro and actin. Arrows indicate the colocalization of SA-Ro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

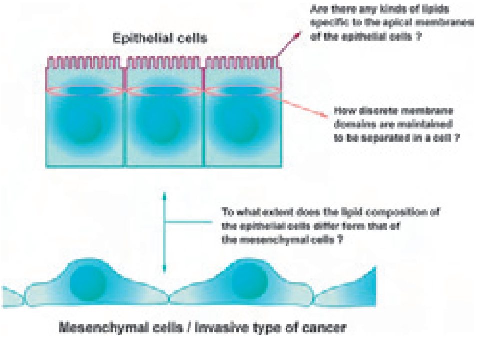


Figure 2.

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 Δ9 position of fatty acyl-CoA substrates, is a rate-limiting enzyme in the biosynthesis of monounsaturated fatty acids (Figure 3A). We generated a series of *Drosophila* mutants that showed a defective expression of stearoyl-CoA desaturase (desat1). One of them, designated *desat1#42*, showed dramatic reduction in TAG content and was defective in survival during starvation (Figure 3B). In the *desat1#42* mutant, the expression of desat1 was specifically reduced in oenocyte, an organ analogous to mammalian liver. The *desat1#42* mutant will provide a unique model for studying the physiological functions of desat1 in energy metabolism.

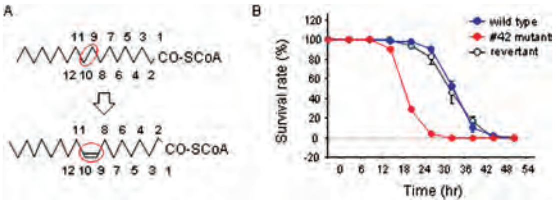


Figure 3. Starvation resistance was reduced in the *desat1#42* mutant flies.
A) Double bond introduction by stearoyl-CoA desaturase.
B) Survival rate of wild type and *desat1#42* mutant flies during starvation.

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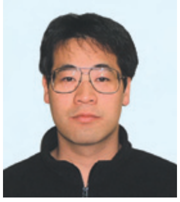
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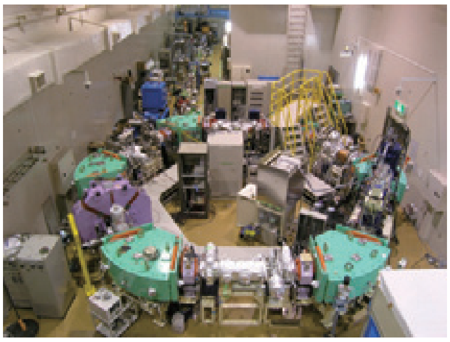
Visitors

Prof KENNEDY, Shane J	Australian Nuclear Science and Tecnology Organization, Australia, 31 January–27 February
Prof SESSLER, Andrew M	Lawrence Berkeley National Laboratory, USA, 30 May–3 June
Prof WEI, Jie	Tsinghua University, China, P. R., 31 May–1 June
Prof GRIESER, Manfred	Max-Planck-Institut für Kernphysik, Germany, 31 May–4 June
Prof JAMESON, Robert A	Goethe University, Germany, 18–20 September

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.

KEYWORDS
Beam Physics
Accelerator Physics
Beam Cooling
Phase Rotation
Neutron Optics



Selected Publications

Noda A, Souda H, Shirai T: Physics of Beam Cooling and Low-temperature Beams, *J. Plasma Fusion Res.*, **86,** 461-465 (2010) (in Japanese).
Iwashita Y, Ichikawa M, Yamada M, Sugimoto T, Tongu H, Fujisawa H, Masuzawa M, Tauchi T, Oku T, Hirota K, Shimizu HM, Shi C, Zhu Y: Practical Applications of Permanent Magnet Multipoles, *IEEE Trans. Appl. Supercond.*, **20,** 842-845 (2010).
Noda A, Souda H, Tongu H, Fujimoto T, Iwata S, Shibuya S, Noda K, Shirai T: Linac Followed by an Electron Cooler to Provide a Short Bunch Proton Beam, *Proc. of the LINAC10*, P1-P3 (2010).
Souda H, Nakao M, Hiromasa T, Tongu H, Noda A, Okamoto H, Smirnov AV, Jimbo K, Grieser M, Shirai T: Transverse Laser Cooling by Synchro-betatron Coupling, *Proc. of IPAC'10*, 861-863 (2010).
Sakaki H, Nishiuchi M, Hori T, Bolton PR, Yogo A, Katagiri M, Ogura K, Sagisaka A, Pirozhkov AS, Orimo S, Kondo K, Iwase H, Niita K, Souda H, Noda A, Iseki Y, Yoshiyuki T: Prompt In-Line Diagnosis of Single Bunch Transverse Profiles and Energy Spectra for Laser-Accelerated Ions, *Appl. Phys. Express*, **3,** 126401(2010).

Collaboration with the Use of Ion Storage and Cooler Ring, S-LSR

ICR has become a collaboration Institute open for outside users. This year, two collaborations has been started.

a) Approach to ultra-low temperature ion beam by laser cooling

We have already obtained an indication of transverse laser cooling of 40 keV $^{24}Mg^+$ ion beam with the use of “Synchro-Betatron Coupling” (Annual Report 2009). This year, more quantitative approach to reach crystalline beam has been triggered by collaboration with the group from Hiroshima University, Tsinghua University and Max-Planck-Institut für Kernphysik through Skype meeting.

b) Irradiation of electron cooled short bunch proton beam onto biological cells

In order to obtain quantitative data on the capability of double strand breaking by irrdadiation of proton beam with a very high peak intensity in a short pulse as indicated by laser-produced proton beam [1], an irradiation system of biological cells by a electron cooled 7 MeV proton beam has been under development. By electron cooling, we have already realized a short bunch 7 MeV proton beam beam with 3.1 ns pulse duration for beam intensity of 1.4 × 10^8 [2]. For the purpose of keeping the cells alive throughout the irradiation process the extracted proton beam is to be deflected vertically as large as 90 degrees and irradiated through a thin foil. By hitting the cells from below, the irradiation condition is expected to be kept constant independent on the thickness of cultivating liquid, which evaporates during the irradiation. Such a beam line is now under construction with collaboration of the group from National Institute of Radiological Sciences.

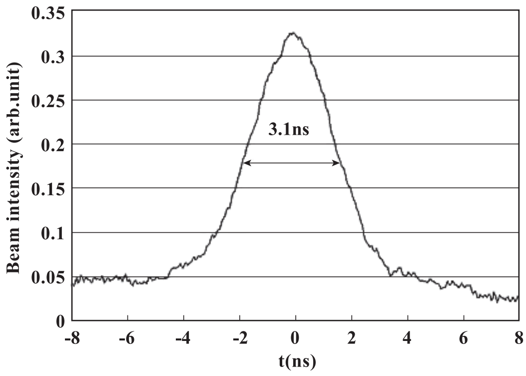


Figure 1. Electron cooled proton beam.

Neutron Optics and Physics (NOP)

Neutron is unique probe for material research and fundamental science because it does not have charge and interacts only by nuclear force, while x-ray interacts with electromagnetic force. Light atoms, which are difficult to be observed by x-rays, can be investigated by neutrons. Among many methods, Small Angle Neutron Scattering (SANS) has been commonly used to investigate structures of materials. Unfortunately, the availability of such facility seems not good because of its huge size (~40 m). By using Very Cold Neutrons (VCN), the length can become very short and be distributed to many laboratories. This situation allows us to invite or raise new neutron users. In addition, wider q-ranges and smaller minimum q’s are available on this VCN-SANS, because the scattering angles are no longer small.

We have been investigating a focusing magnetic lens for neutrons that has sextupole magnetic field to interacts with magnetic dipole moment of neutrons. The focusing properties were studied at ILL, Grenoble, France. Figure 2 shows the typical results. Using this lens, test measurements of VCN-SANS were performed. Figure 3 shows the result for tri-block-copolymer case. The resolution Figure 3 was better than the conventional facility. We are still studying towards the better performance.

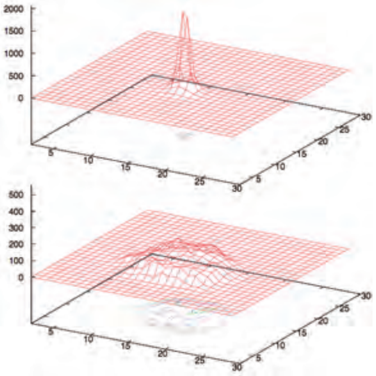


Figure 2. The beam profiles on the 2D detector. Top: PMSx is well synchronized and the beam spot is kept small during the beam pulse. Bottom: the beam spot is increasing for off-synchronized case.

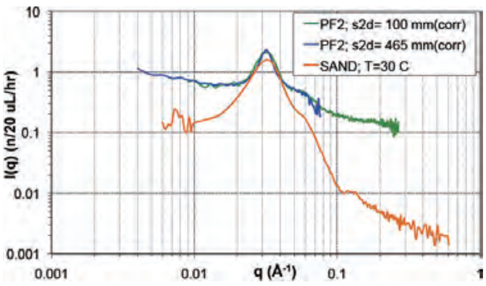


Figure 3. VCN-SANS plots for 15 wt% Pluronic in D2O (28 °C), compared with SAND@IPNS.

References
[1] A. Yogo et al., Appl. Phys. Lett. **94,** 181502 (2009).
[2] T. Fujimoto et al., N.I.M. **A588,** 330-335 (2008).

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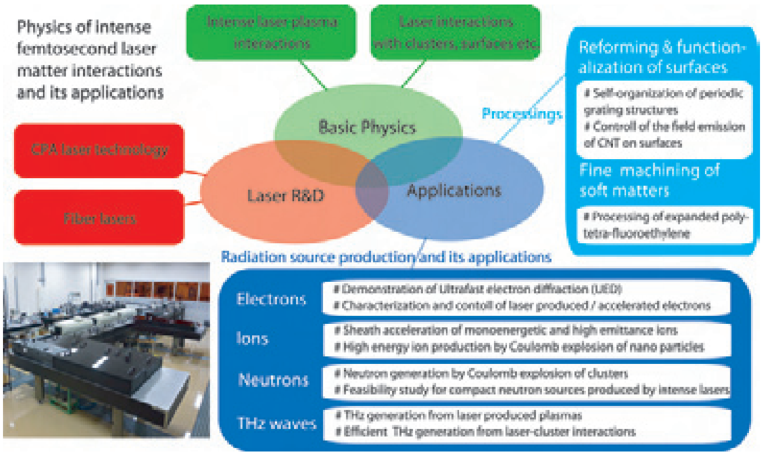
Scope of Research

The interaction of femtosecond laser pulses with matters involves interesting physics, which does not appear in that of nanosecond laser pulses. Investigating the interaction physics, potential of intense femtosecond lasers for new applications is being developed (such as laser produced radiations and laser processing). Ultra-intense lasers can produce intense radiations (electrons, ions, THz, and so on), which can be expected as the next-generation radiation sources. Ultra-short lasers are available to process any matters without thermal dissociation. The femtosecond laser processing is also the next-generation laser processing. In our laboratory ultra intense femtosecond laser named T^6-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

KEYWORDS

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



Selected Publications

Inoue S, Tokita S, Nishoji T, Masuno S, Otani K, Hashida M, Sakabe S: Single-shot Microscopic Electron Imaging of Intense Femtosecond Laser-produced Plasmas, *Rev. Sci. Instrum.*, **81,** 123302 (2010).

Tokita S, Hirokane M, Murakami M, Shimizu S, Hashida M, Sakabe S: Stable 10 W Er:ZBLAN Fiber Laser Operating at 2.71–2.88 μm, *Opt. Lett.*, **35,** 3943 (2010).

Tokita S, Hashida M, Inoue S, Nishoji T, Otani K, Sakabe S: Single-Shot Femtosecond Electron Diffraction with Laser-Accelerated Electrons: Experimental Demonstration of Electron Pulse Compression, *Phys. Rev. Lett.*, **105,** 215004 (2010).

Okamuro K, Hashida M, Miyasaka Y, Ikuta Y, Tokita S, Sakabe S: Laser Fluence Dependence of Periodic Grating Structures Formed on Metal Surfaces under Femtosecond Laser Pulse Irradiation, *Phys. Rev. B*, **82,** 165417 (2010).

Hashida M, Namba S, Okamuro K, Tokita S, Sakabe S: Ion Emission from a Metal Surface through a Multiphoton Process and Optical Feld Ionization, *Phys. Rev. B*, **81,** 115442 (2010).

Periodic Grating Structures Self-formed on Metal Surfaces under Femtosecond Laser Pulse Irradiation

Periodic structures self-formed on the surface of several metals by femtosecond laser pulses are investigated by electron microscopy. For the self-formation of periodic gratings on metal surfaces, the interspaces of the periodic structures depend on laser fluence. This dependence is the same for all metals, although the range of laser fluence in which the structures are formed differs between metals (Figure 1). The laser fluence dependence can be explained by the generation of a plasma wave through the parametric decay of laser light [Phys. Rev. B 79, 033409(2009)]. This indicates that the formation of periodic structures depends not on metal properties, but only on the electron density of plasma produced on a surface by femtosecond laser pulses.

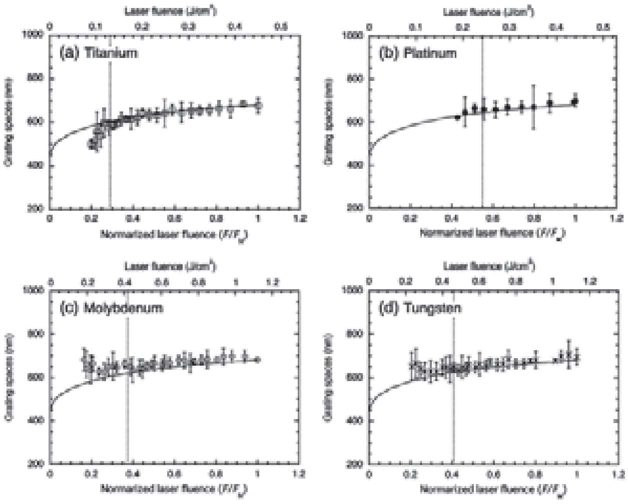


Figure 1. Laser fluence dependence of the periodic structure interspaces produced by femtosecond laser pulses for (a) Ti, (b) Pt, (c) Mo, and (d) W (pulse duration: 160 fs). The interspace of the grating structure was determined by analyzing a set of 10 irradiated spots on the metal surface. Error bars show the standard deviation of the interspaces. Laser fluence is normalized by the upper limit on laser fluence for producing periodic structures, F_M. Solid lines show calculation results according to the parametric decay model proposed by Sakabe *et al.*, and dotted lines show the laser fluence for the ablation rate of 10 nm/pulse.

Femtosecond Pulse Compression of Laser-accelerated Electron Pulses

Time-resolved electron diffraction and microscopy using femtosecond electron pulses is a powerful method for observing atomic-scale ultrafast structural changes. Such an advanced method is crucial for the study of ultrafast phenomena in a broad range of scientific fields, including physics, chemistry, materials science, and biology, because the method enables the direct observation of atomic processes. However, due to the space-charge effect, the brightness of probe electron pulses is low and insufficient in most cases using conventional electron guns.

We have developed a new method for solving the space-charge problem in ultrafast electron diffraction. This unique method involves compression an intense laser-accelerated electron pulse. Figure 2 shows the femtosecond electron-pulse generation system. Accelerated by a femtosecond laser pulse with an intensity of 10^{18} W/cm^2, an electron pulse with an energy of around 350 keV and a relative momentum spread of about 1% was compressed to a 500-fs pulse at a distance of about 50 cm from the electron source by using a magnetic pulse compressor. Furthermore, the electron pulse was used to generate a clear diffraction pattern of a gold crystal in a single shot. This technique has great potential for the generation of extremely high-charge femtosecond pulses in the sub-MeV range, because the space-charge effect does not limit the charge in a pulse. We expect that this development will fundamentally change the observation of ultrafast phenomena by electron pulses in the near future.

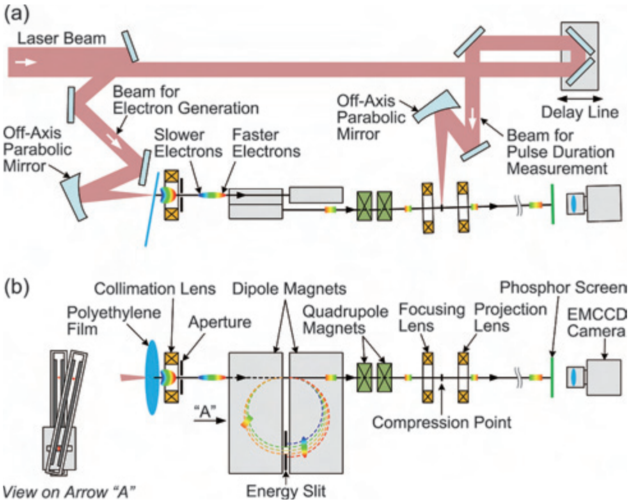


Figure 2. Schematic diagram of the experimental setup of electron pulse compression and pulse duration measurement: (a) top view and (b) side view. Everything except the EMCCD camera is operated in a vacuum at 10^{-2} Pa.

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Visitors

Prof VALMALETTE, Jean-Christophe	Université du Sud Toulon Var, France, 19 February
Prof CHAIRUANGSRI, Torranin	Chiang Mai University, Thailand, 15–31 March
Prof Em EGERTON, Raymond F.	University of Alberta, Canada, 5 April
Dr LO, Shen-Chuan	Industrial Technology Research Institute, Taiwan, 26–29 April
Dr CHEN, Shih-Yun	National Taiwan University of Science and Technology, Taiwan, 20 July
Dr GLOTER, Alexandre	Laboratoire de Physique des Solides (CNRS), France, 23 August
Dr LAI, Ming-Wei	Industrial Technology Research Institute, Taiwan, 6–9 September

Scope of Research

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

KEYWORDS

TEM
STEM
Cryo-TEM
EELS
SPM

Selected Publications

Kobayashi T, Ogawa T, Moriguchi S, Suga T, Yoshida K, Kurata H, Isoda S: Inhomogeneous Substitution of Polyhalogenated Copper-phthalocyanine Studied by High-resolution Imaging and Electron Crystallography, *J. Electron Microsc.*, **52,** 85-90 (2003).

Minari T, Nemoto T, Isoda S: Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor, *J. Appl. Phys.*, **99,** 034506 (2006).

Kiyomura T, Nemoto T, Ogawa T, Minari T, Yoshida K, Kurata H, Isoda S: Thin-Film Phase of Pentacene Film Formed on KCl by Vacuum Deposition, *Jpn. J. Appl. Phys.*, **45,** 401-404 (2006).

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

Haruta M, Kurata H, Komatsu H, Shimakawa Y, Isoda S: Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite La_2CuSnO_6, *Physical Review B*, **80,** 165123 (2009).

HRTEM and ADF-STEM of Precipitates in Aluminium Alloy

Precipitates at peak-ageing in an A356 Al–Mg–Si alloy cast by a semi-solid process have been studied by high-resolution transmission electron microscopy (HRTEM) and annular dark-field scanning transmission electron microscopy (ADF-STEM). The precipitate most frequently found in the alloy is the β” phase (Mg_5Si_6) or its precursors. Although the contrast of ADF image, especially HAADF, an atom with a higher atomic number should show a brighter contrast comparing to one with a lower atomic number (Z-contrast), the precipitate shows the darker contrast as compared to that of the Al matrix in High Angle ADF-STEM (HAADF-STEM), and vice versa in Low Angle ADF-STEM (LAADF-STEM). To understand such contrast, a dynamical simulation based on the multi-slice method was performed using different atomic stacking models; the precipitate layer is located at the top (I), bottom (II) or middle (III) of the sample. Model (III), where the precipitate situates inside the Al matrix, successfully explained the reverse contrast of the experimental images of the precipitate. The origin of such a strange contrast variation comes from the dynamical and the channeling effects in the crystalline precipitate situated in a crystalline matrix, of which the dynamical simulation is indispensable in structure analysis. The LAADF-STEM is a potential tool in atomic structure analysis of precipitates in combination with HAADF-STEM.

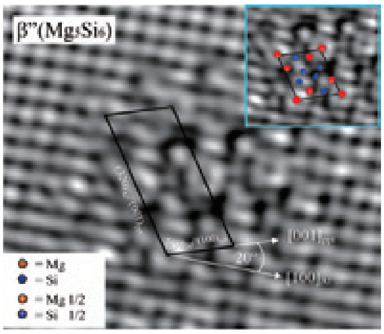

Figure 1. Noise-filtered HRTEM image of the precipitate.

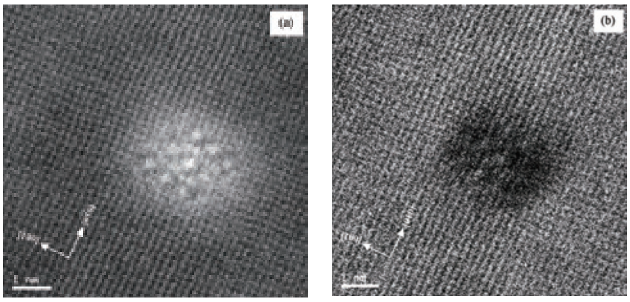

Figure 2. LAADF (a) and HAADF (b) images of the same precipitate.

Gelation Behavior by the Lanthanoid Adsorption of the Cyanobacterial Extracellular Polysaccharide Sacran

Cyanobacteria, which live in the rivers and sea where industrial waste is discharged, produce and secrete polysaccharides with functional groups such as carboxylic acid, sulfates, phosphates and amines that are responsible for ionic adsorption. These extracellular polysaccharides adsorb heavy metal ions in the water to prevent toxicity, and protect the cells themselves. The self-organization behavior of an extracellular polysaccharide (sacran) extracted from the cyanobacterium Aphanothece sacrum in response to lanthanoid ion adsorption was investigated. Cryo-TEM images revealed that sacran could be cross-linked by trivalent metal ions, and formed a fibrous nano structural network containing water. The network structure of the nanoconstructs was formed to construct macroscopic gels. The critical gelation concentrations of sacran were very low. These findings strongly suggest that the extracellular matrix of Aphanothece sacrum was gelated efficiently by the sacran associating to form nanonetworks of metal-complex fibers, which reinforced the jelly matrix. This may represent a strategy of Aphanothece sacrum for protecting their own cell bodies from external biological and physical stimuli.

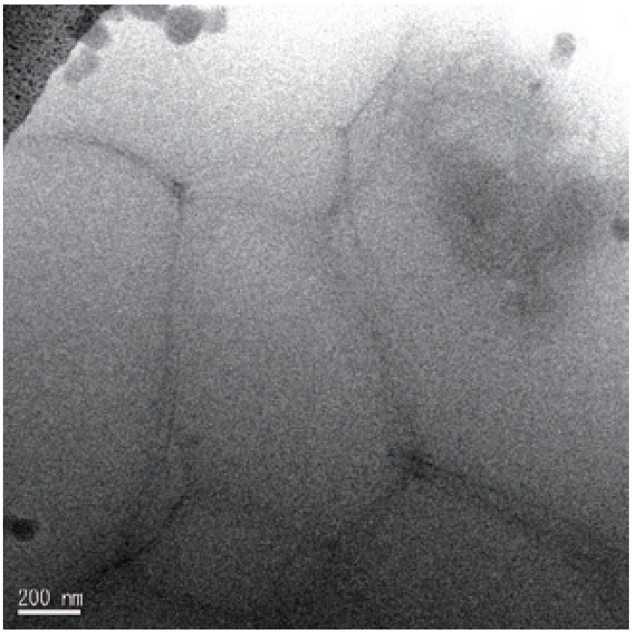

Figure 3. Cryo-TEM image of quick-frozen samples of a dispersed solution of sacran into $NdCl_3$ solution.

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OKAMOTO, Shigeki (M1)
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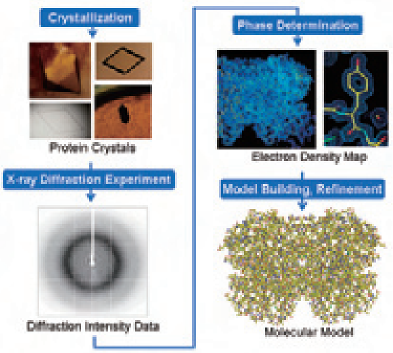
Scope of Research

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-Xα and WIEN2k, and the development of new typed X-ray spectrometer with ultra high-resolution have also been carried out.

KEYWORDS
Crystal
X-ray Crystallographic Analysis
Maleylacetate Reductase
Resorcinol Catabolism
Enzymatic Reaction



Selected Publications

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

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

Open and Closed Subunit Structures of *Rhizobium* Maleylacetate Reductase

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. Therefore, much attention has been paid to the *Rhizobium* genes and gene products for their role in the regulation of symbiosis. Despite extensive studies on *Rhizobium*, 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 as a microorganism with a high level of γ-resorcylate (2,6-hydroxybenzoate) decarboxylase (EC 4.1.1.x) activity. During the cloning of the *graF* gene encoding the enzyme γ-resorcylate decarboxylase, the genes *graA*, *graB*, *graC*, and *graD* were found immediately upstream and downstream of *graF*. Enzymological studies showed that *graD*, *graA*, *graB*, and *graC* encode the reductase (GraD) and oxidase (GraA) components of resorcinol hydroxylase (EC 1.14.13.x), hydroxyquinol 1,2-dioxygenase (GraB) (EC 1.13.11.37), and maleylacetate reductase (GraC) (EC 1.3.1.32), 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 crystal was prepared by the sitting-drop vapour-diffusion method complemented with a microseeding technique. Good crystals were obtained at 293 K in 3days with protein solution at 8 mg/ml (in 50 mM Tris-HCl buffer, pH 8.0) and 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 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 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. 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 Rfree=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 (Subunit-A & Subunit-B) have a little bit different structures from each other in the present crystal. The difference is clear by superposing two subunits based on not only whole subunit but also each domain (Figure 1). Superposition of the two subunits based on the corresponding Cα atoms for whole subunits, N-terminal domain region, and C-terminal domain region show the values of root means square deviations of 1.93 Å, 0.79 Å, and 0.52 Å, respectively. Subunit-A 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. Subunit-B 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. The active site structure of GraC shows several histidines residues in the cleft, some of which interact with binding sulfate anion (Figure 2). This suggests that these histidine residues may be involved in the enzymatic reaction or ligand binding.

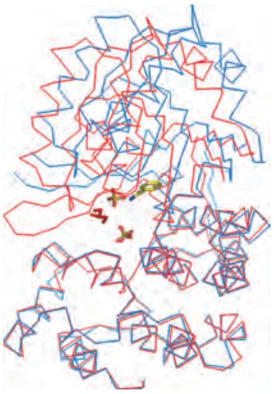

Figure 1. Superposition of GraC subunits. Subunit-A and Subunit-B are shown in red and blue, respectively.

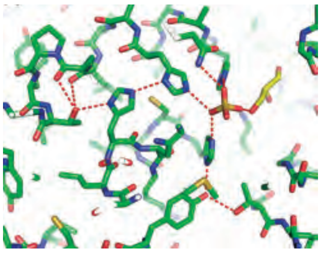

Figure 2. Active site structure of GraC. The dash lines represent hydrogen-bonds.

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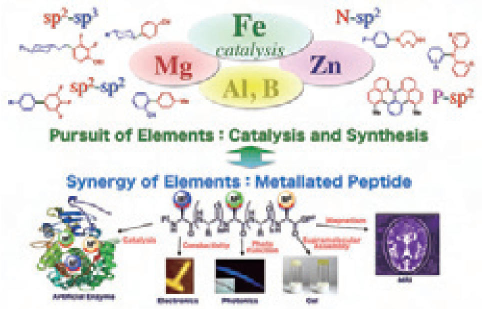
Prof LEE, Hee-Seung	Korea Advanced Institute of Science and Technology, KAIST, Korea, R., 23 February
Prof SHING, Tony K M	Department of Chemistry, The Chinese University of Hong Kong, Hong Kong, China, P. R., 1 June–31 August
Prof MAZET, Clement	Department of Organic Chemistry, University of Geneva, Geneva, Switzerland, 9 July
Prof DOUCET, Henri	Institut Sciences Chimiques de Rennes, Université de Rennes, Catalyse et Organometalliques, Rennes, France, 12 July
Prof ORGAN, Michael G	Department of Chemistry, York University, Toronto, Canada, 8 November

Scope of Research

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



KEYWORDS

Carbon–Carbon Bond Formation
Iron Catalyst
Cross-Coupling Reaction
Metallated Peptide
π-Conjugated Molecule

Selected Publications

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

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

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

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,** 11949-11963 (2009).

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

Diastereoselective Carbometalation of Oxa- and Azabicyclic Alkenes under Iron Catalysis

Transition-metal-catalyzed carbometalation of alkenes is a powerful synthetic tool for selective carbon–carbon bond formation. Through sequential electrophilic trapping of the intermediate organometallic species, regio- and stereoselective construction of contiguous *sp*^{3} carbon centers can be achieved in a single-pot procedure. We have developed the iron-catalyzed highly diastereoselective carbometalation of various oxa- and azabicyclic alkenes with arylzinc reagents. The carbozincation products were quenched with acid or trapped with electrophiles, giving the corresponding products in excellent yield. Among a series of novel DPPBz derivatives, electron-deficient ligand was found particularly effective to facilitate the carbometalation and suppress the β-heteroatom elimination.

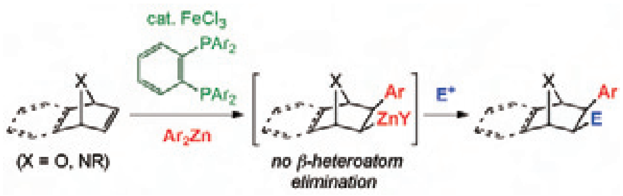


Figure 1. Iron-Catalyzed Diastereoselective Carbozincation of Oxa- and Azabicyclic Alkenes.

Nickel-Catalyzed Alkenylative Cross-Coupling Reaction of Alkyl Sulfides

Transition metal-catalyzed cross-coupling reactions are powerful tools in organic synthesis. While various electrophilic substrates have been utilized in the cross-coupling reactions, organosulfur compounds have received far less attention among them in spite of the long history. In light of the ample supply of sulfur sources, especially as by-products of refinery, in industrial chemistry, we have explored new reactivity of organosulfur compounds in the cross-coupling reaction and found that alkyl aryl sulfides act as *alkenyl* electrophiles to give the arylation products with the simultaneous installation of an olefinic part in the products. The key to success is the use of a bulky NHC ligand, SIPr, which suppresses the conventional biaryl coupling reaction. The theoretical calculation suggests a concerted mechanism for the *β*-hydride elimination and reductive elimination process from nickel(II) thiolate species, which accounts for the new reactivity of the organosulfur electrophile in the present alkenylative cross-coupling.

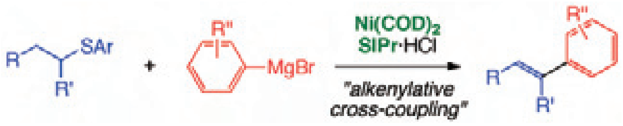


Figure 2. Nickel-Catalyzed Alkenylative Cross-Coupling Reaction.

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

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

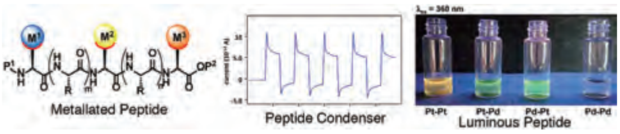


Figure 3. Preparation of Metallated Peptide and Self-Assembly of the Peptide.

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Visitors

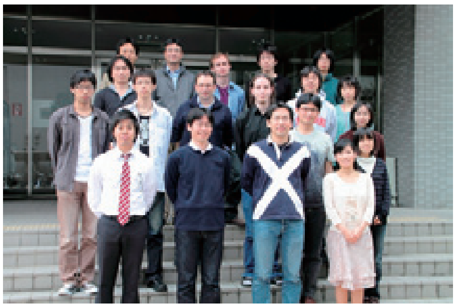
Assoc Prof VALANOOR, Nagarajan	University of New South Wales, Australia, 22 January
Dr KOLESNIKOV, Alexander I.	Oak Ridge National Laboratory, USA, 30 January
Prof WILEY, John B.	University of New Orleans, USA, 1 March
Prof ATTFIELD, J. Paul	University of Edinburgh, UK, 15 March
Prof PAULUS, Werner	University of Rennes 1, France, 25 March
Prof LOYE, Hans-Conradzur	University of South Carolina, USA, 24 May
Prof TAKEUCHI, Ichiro	University of Maryland, USA, 8 July
Assoc Prof HEMANDEZ, Olivier	University of Rennes 1, France, 27 July

Scope of Research

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

KEYWORDS

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



Selected Publications

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

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

Anisotropic Oxygen Diffusion at Low Temperature in Perovskite Structure Iron Oxides

Oxygen-ion conduction in transition-metal oxides has been extensively investigated due to its potential of device applications such as electrolytes in solid-oxide fuel cells and oxygen-separation membranes. However the operation temperature is currently limited to only high temperature region. Achieving enough oxygen ion conduction at lower temperature is, therefore a key to further developments of the oxygen-ion conduction based devices. Furthermore an understanding of the oxygen-diffusion pathways in the oxides would provide ideas on ideal structures that allow the efficient ion conduction at lower temperatures.

Here we report that brownmillerite-structured $CaFeO_{2.5}$ epitaxial thin films undergo a structural change into $CaFeO_2$ with an infinite-layer structure (Figure 1) through low-temperature reductions with CaH_2.

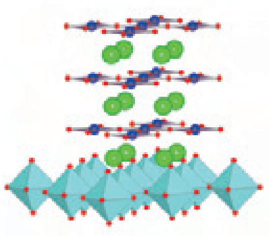


Figure 1. Schematic infinite-layer structure $CaFeO_2$ on a substrate.

We found that some of the oxygen atoms are released from the perovskite-structure framework and others are rearranged within it during the reduction process. Both the observed structural changes and the reaction time necessary for the reduction process on the film orientations show the strong dependence on the film orientations. This reveals two oxygen diffusion pathways and the related kinetics at low temperature. These results demonstrate that oxygen diffusion in the brownmillerite is highly anisotropic, significantly higher along the lateral direction of the tetrahedral and octahedral layers as shown in Figure 2.

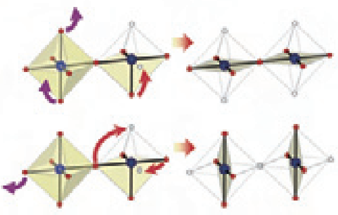


Figure 2. Schematics of two types of oxygen diffusion pathways and the rearrangement from tetrahedral to square-planar coordination in FeO_4.

Charge Transfer and Antiferromagnetic Order in The A-site-ordered Perovskite $LaCu_3Fe_4O_{12}$

A-site-ordered double perovskite oxides with the general formula $AA'_3B_4O_{12}$ have attracted enormous interest owing to their wide variety of physical properties. Recently we found a novel A-site-ordered double perovskite oxides $LaCu_3Fe_4O_{12}$ displaying a temperature-induced intersite charge transfer. This charge transfer is attributed to the simultaneous valence changes between the A' and B sites, namely $3Cu^{2+} + 4Fe^{3.75+} \rightarrow 3Cu^{3+} + 4Fe^{3+}$ where the paramagnetic metallic phase at higher temperature transforms to the antiferromagnetically-ordered insulating phase at lower temperature. In this study we employed high resolution neutron powder diffraction to investigate the charge states and spin order in this compound. We found that a first-order phase transition takes place at T_{CT} ~400 K between cubic *Im*-3 structures with charge distributions $LaCu^{3+}{}_3Fe^{3+}{}_4O_{12}$ and $LaCu^{2+}{}_3Fe^{3.75+}{}_4O_{12}$. Bond valence sums confirm that these charge states are adopted in the two phases, and there are no substantial valence fluctuations near the charge transfer transition. G-type antiferromagnetic order of Fe^{3+} spins at the B-site is observed in the low temperature phase $LaCu^{3+}{}_3Fe^{3+}{}_4O_{12}$ and the ordered moment at 50 K is 4.0 μ_B. Magnetic moment is absent at the A'-site Cu^{3+} cation. The thermal evolution of the ordered moment enables an intrinsic $T_{N'}$ ~ 600 K to be estimated, although the actual upper limit for the spin order is T_{CT} (Figure 3). No long range magnetic ordering is also found in the high temperature phase, $LaCu^{2+}{}_3Fe^{3.75+}{}_4O_{12}$, showing that any ordering transition for this regime has $T_M < T_{CT}$.

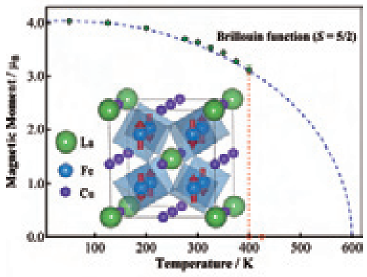


Figure 3. Temperature dependence of the refined Fe^{3+} magnetic moment at the B-site in $LaCu_3Fe_4O_{12}$.The inset shows the crystal structure of the low temperature phase with G-type antiferromagnetic ordering.

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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, and (2) preparation of π-conjugated polymers by the use of well defined cross-coupling reactions.

KEYWORDS
Transition Metal Complex
Homogeneous Catalyst
Reaction Mechanism
Synergistic Effect

Selected Publications

Wakioka M, Ikegami M, Ozawa F: Stereocontrolled Synthesis and Photoisomerization Behavior of All-cis and All-trans Poly(m-phenylenevinylene)s, *Macromolecules*, **43,** 6980-6985 (2010).

Wang Q, Takita R, Kikuzaki Y, Ozawa F: Palladium-Catalyzed Dehydrohalogenative Polycondensation of 2-Bromo-3-hexylthiophene: An Efficient Approach to Head-to-Tail Poly(3-hexylthiophene), *J. Am. Chem. Soc*., **132,** 11420-11421 (2010).

Nakajima Y, Nakao Y, Sakaki S, Tamada Y, Ono T, Ozawa F: Electronic Structure of Four-coordinate Iron(I) Complex Supported by a Bis(phosphaethenyl)pyridine Ligand, *J. Am. Chem. Soc*., **132,** 9934-9936 (2010).

Wakioka M, Ozawa F: Substituent Effects on P-C Reductive Elimination from Styrylpalladium(II) Phosphine Complexes, *Organometallics*, **29,** 5570-5578 (2010).

Nakajima Y, Nakatani M, Hayashi K, Shiraishi Y, Takita R, Okazaki M, Ozawa F: Synthesis and Structures of Platinum Diphenylacetylene and Dithiolate Complexes Bearing Diphosphinidenecyclobutene Ligands (DPCB-Y), *New. J. Chem*., **34,** 1713-1722 (2010).

Substituent Effects on P–C Reductive Elimination from Styrylpalladium(II) Phosphine Complexes

While the P–C reductive elimination of hydrocarbyl and phosphine ligands is frequently observed, its mechanistic information has been limited. In this work, we prepared a series of styryl palladium complexes **1**, having a series of para substituents with different electronic properties on Ar and Ar' groups, and examined their reductive elimination in the presence of added PMeAr'$_2$ by kinetic experiments. The kinetic data are consistent with the reaction process involving prior association of **1** with PMeAr'$_2$ to form a five-coordinate intermediate (**A**), which subsequently undergoes P–C reductive elimination to give **2**. The rate constant for P–C reductive elimination (k) increases to a great extent as the electron-donating ability of para substituents increases, and showed a good Hammett correlation with the σ_p values of substituents [ρ = –2.43 and –4.8 (for Ar and Ar', respectively)].

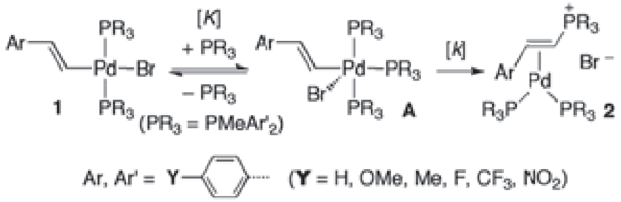

Figure 1. P−C reductive elimination from **1** in the presence of added PMeAr'$_2$.

Palladium-Catalyzed Dehydrohalogenative Polycondensation of 2-Bromo-3-hexylthiophene: An Efficient Approach to Head-to-Tail Poly(3-hexylthiophene)

Poly(3-alkylthiophene)s are among the most promising π-conjugated polymers for the development of flexible electronic devices. It has been documented that their physical properties are strongly affected by the regioregularity of the thiophene units, and head-to-tail polymers are superior to regiorandom isomers. In this work, we examined the synthesis of head-to-tail poly(3-hexylthiophene) (HT-P3HT) using palladium-catalyzed dehydrogenative polycondensation of 2-bromo-3-hexylthiophene (**3**). The reaction of **3** with **4** and **5** as catalyst precursors gave HT-P3HT with high molecular weight (M_n = 30600, M_w/M_n = 1.60) and high regioregularity (98%) in almost quantitative yield (99%). This process, which does not require prepreparation of organometallic reagents, should be of benefit with respect to reduced waste generation and fewer reaction steps.

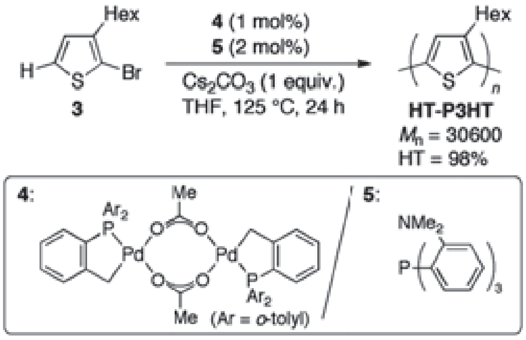

Figure 2. Palladium-catalyzed dehydrohalogenative polycondensation of 2-bromo-3-hexylthiophene (**3**).

Electronic Structure of Four-coordinate Iron(I) Complex Supported by a Bis(phospha ethenyl)pyridine Ligand

A 15-electron iron complex with a formal Fe(I) center, [FeBr(BPEP)] (BPEP = 2,6-bis(1-phenyl-2-phosphaethenyl) pyridine), was prepared by one-electron reduction of the dibromide precursor [FeBr$_2$(BPEP)]. The single-crystal diffraction analysis revealed a distorted trigonal monopyramidal arrangement around the iron center. DFT calculations for a model complex revealed two highly delocalized molecular orbitals formed by bonding and antibonding interactions between the d_{z2} (Fe) and π* (BPEP) orbitals. Orbital occupancy analysis demonstrated the electronic structure with a high-spin Fe(I) center. The effective interaction between iron and BPEP was concluded to be responsible for the highly distorted structure of [FeBr(BPEP)], with its rather uncommon trigonal monopyramidal configuration.

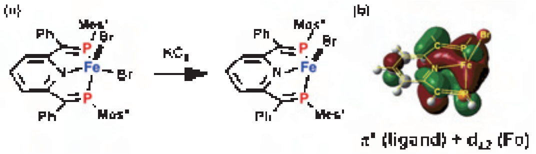

Figure 3. (a) Formation of [FeBr(BPEP)], (b) delocalized molecular orbital of [FeBr(BPEP)].

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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.

KEYWORDS
Femtosecond Laser Spectroscopy
Carbon Nanotube
Semiconductor Nanoparticles
Transition Metal Oxides
Semiconductor Nanostructures

Selected Publications

Yamada Y, Yasuda H, Tayagaki T, Kanemitsu Y: Temperature Dependence of Photoluminescence Spectra of Undoped and Electron-doped $SrTiO_3$: Crossover from Auger Recombination to Single-carrier Trapping, *Phys. Rev. Lett.*, **102,** [247401-1]-[247401-4] (2009).

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

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

Ito Y, Matsuda K, Kanemitsu Y: Mechanism of Photoluminescence Enhancement in Single Semiconductor Nanocrystals on Metal Surfaces, *Phys. Rev. B*, **75,** [033309-1]-[033309-4] (2007).

Hirori H, Matsuda K, Miyauchi Y, Maruyama S, Kanemitsu Y: Exciton Localization of Single-walled Carbon Nanotubes Revealed by Femtosecond Excitation Correlation Spectroscopy, *Phys. Rev. Lett.*, **97,** [257401-1]-[257401-4] (2006).

Band-to-band Photoluminescence in $SrTiO_3$

Transition metal oxides have attracted a great deal of attention as new device materials due to their wide variety of fascinating and multifunctional properties. $SrTiO_3$ is one of the most important oxide materials. We observed band-edge photoluminescence (PL) in highly photoexcited $SrTiO_3$ and electron-doped $SrTiO_3$ at low temperatures. Two band-edge PL peaks coincide with the low- and high-temperature onsets of optical absorption. This clearly shows that band-edge PL peaks correspond to indirect band-to-band radiative recombination involving phonon emission and absorption processes and allows a determination of the band gap.

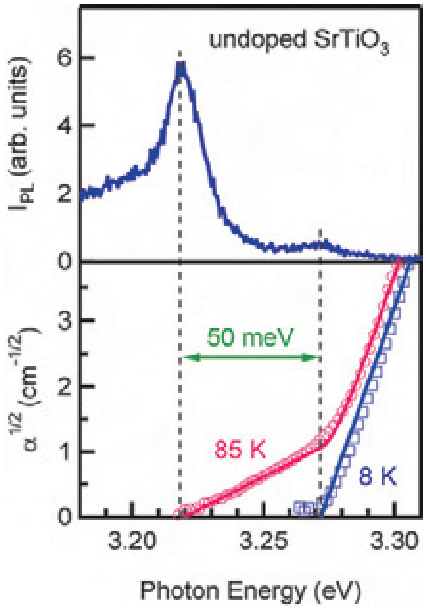

Figure 1. Time-gated (0–8 ns) PL spectrum of $SrTiO_3$ at 8 K (upper) and the square root of the absorption coefficient at 8 and 85 K (lower).

Multicarrier Recombination and Energy Transfer in Mn-Doped CdS Nanocrystals Studied by Femtosecond Pump-Probe 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 the photocarrier decay dynamics of Mn-doped CdS NCs coated with a ZnS shell layer by femtosecond pump–probe transient absorption spectroscopy. At low excitation intensities, the decay dynamics of photocarriers is determined by energy transfer from electron–hole pairs in CdS NCs to Mn ions. At high excitation intensities, the photocarrier decay curves of Mn-doped CdS NCs are very similar to those of undoped CdS NCs, and they are determined by the fast Auger recombination of photocarriers. These density-dependent photocarrier behaviors in CdS NCs are confirmed by Mn^{2+} luminescence spectroscopy.

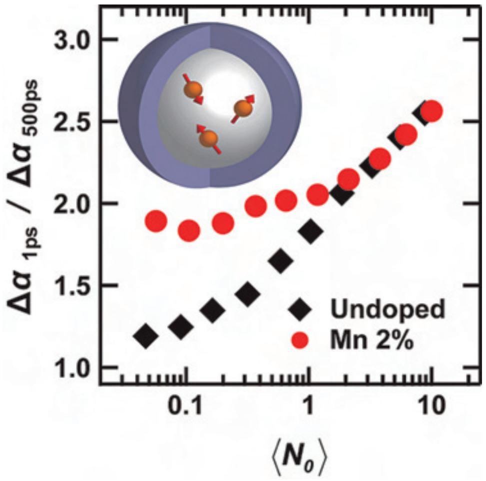

Figure 2. Intensity ratio of the transient absorption signal at 1 ps to that at 500 ps as a function of the average number of initially photocreated e–h pairs.

Plasmon-assisted Photoluminescence Enhancement of Single-Walled Carbon Nanotubes on Metal Surfaces

Carbon nanotubes are one of the excellent materials for studying the optical properties of excitons, because of their unique band structures and large exciton binding energies. We demonstrated PL enhancement in single carbon nanotubes using localized surface plasmons. Single nanotube spectroscopy revealed triple the PL intensity enhancement for carbon nanotubes on rough Au surfaces as on fused silica surfaces. The PL enhancement depends on the excitation wavelength and distance between the carbon nanotubes and the Au surface. The degree of PL enhancement is determined by the electric field enhancement from the localized surface plasmon and the energy transfer from the carbon nanotube to the metal surface.

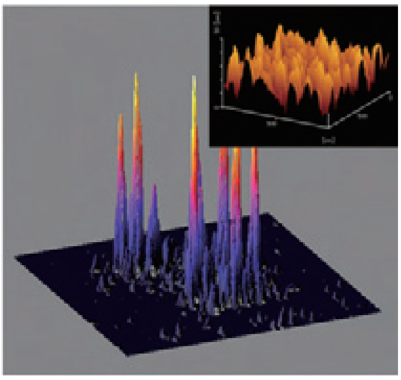

Figure 3. PL images of single carbon nanotubes on the rough Au surfaces. The image size is 40×40 μm^2. Inset: Topographic images of rough and flat Au surfaces measured using atomic force microscopy with a vertical scale of ±25 nm and area of 1×1 μm^2.

Bioinformatics Center
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Visitors

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Assist Prof	RAMIREZ-PRADO, Jorge H	Scientific Research Center of Yucatan (CICY), Mexico, 7 June–31 August 2010

Scope of Research

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

KEYWORDS
KEGG
(Meta)genomics
Pathway
Bioinformatics
Metabolomics

Selected Publications

Hattori M, Tanaka N, Kanehisa M, Goto S: SIMCOMP/SUBCOMP: Chemical Structure Search Servers for Network Analyses, *Nucleic Acids Res.*, **38,** W652-W656 (2010).

Moriya Y, Shigemizu D, Hattori M, Tokimatsu T, Kotera M, Goto S, Kanehisa M: PathPred: An Enzyme-catalyzed Metabolic Pathway Prediction Server, *Nucleic Acids Res.*, **38,** W138-W143 (2010).

Diez D, Hayes N, Joannin N, Normark J, Kanehisa M, Wahlgren M, Wheelock CE, Goto S: varDB: A Database of Antigenic Variant Sequences — Current Status and Future Prospects, *Acta Trop.*, **14,** 144 (2010).

Kanehisa M, Goto S, Furumichi M, Tanabe M, Hirakawa M: KEGG for Representation and Analysis of Molecular Networks Involving Diseases and Drugs, *Nucleic Acids Res.*, **38,** D355-D360 (2010).

Wheelock CE, Wheelock AM, Kawashima S, Diez D, Kanehisa M, van Erk M, Kleemann R, Haeggstrom JZ, Goto S: Systems Biology Approaches and Pathway Tools for Investigating Cardiovascular Disease, *Mol. Biosyst.*, **5,** 588-602 (2009).

RCLASS: Reaction Class Database

Recent development of high-throughput measurement techniques has put omics research (genomics, proteomics, metabolomics, etc.) forward to analysis on organism communities. For example, next-generation sequencers are expected to be powerful to analyze environmental genomics, also referred to as “metagenomics”. Similarly, high-throughput mass spectrometry enables to analyze metabolomics on organism communities, referred to as “meta-metabolomics”.

Our future goal is the integration of metagenomics and meta-metabolomics, i.e., linking metagenomic information to the interconversion among the chemical substances from environment. We developed the E-zyme software for the initial step to elucidate enzymes for a partial reaction equation. E-zyme is reaction types named as the RDM chemical transformation patterns. Specific RDM patterns are uniquely and preferentially found in specific categories of the KEGG metabolic pathways. We developed KEGG RCLASS database, classification of reactions based on the RDM patterns of reactions on metabolic pathways. One can consider the relationships between enzyme reaction similarity and enzyme protein similarity even the reaction equation is only partially identified, thus RCLASS is proposed to be beneficial to link meta-metabolomics to metagenomics, as well as to analyze consecutive reaction patterns conserved in the evolution of metabolic pathways.

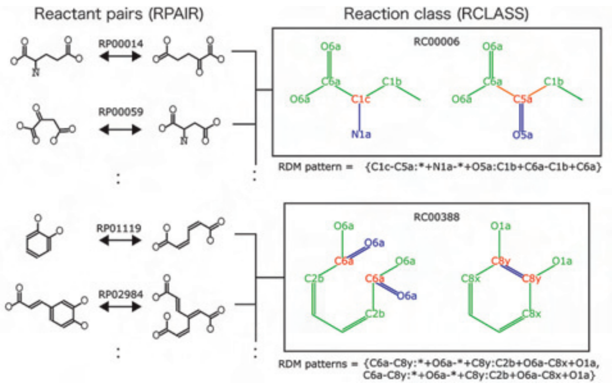


Figure 1. Example RCLASS entries and the RPAIR members.

PathPred: Enzyme-Catalyzed Reaction Pathway Prediction

PathPred is a newly developed web tool to predict plausible multi-step enzyme-catalyzed reaction pathways from a query compound using the information of the biochemical transformation patterns (RDM patterns) and chemical structure alignments of substrate-product pairs. PathPred provides transformed compounds and reference transformation patterns in each predicted reaction, and displays all predicted multi-step reaction pathways in a tree-shaped graph. This prediction server focuses on microbial biodegradation of environmental compounds and biosynthesis of plant secondary metabolites.

PathPred is a fully automatic server repeating prediction cycles until they reach the pre-specified compound, which is given by the user or is a compound present in the KEGG metabolic pathway maps. Another unique feature of PathPred is its potential to link the prediction result to genomic information. The PathPred server reports new and alternative reaction steps irrespective of whether enzymes for these steps are known or not. If the enzyme is not known, the E-zyme tool may be used to assign a possible EC number, which may then be used to search possible genes by sequence similarity of known genes.

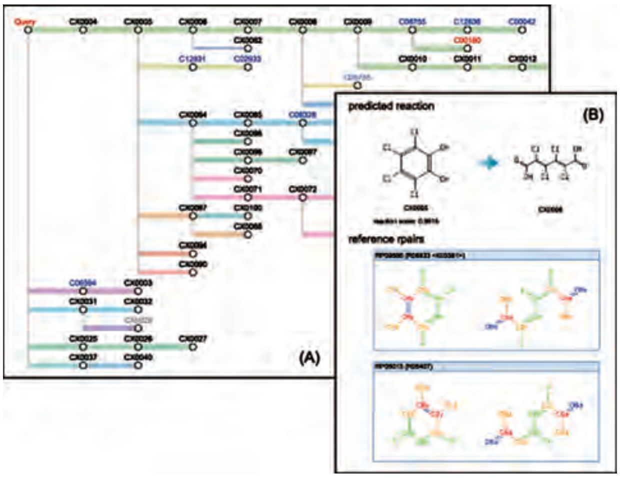
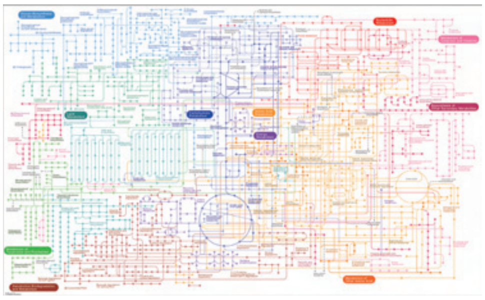


Figure 2. The example of the predicted pathway tree (A) and predicted reaction with referenced reactions.



Bioinformatics Center
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LAI, Yeuntyn (M1)
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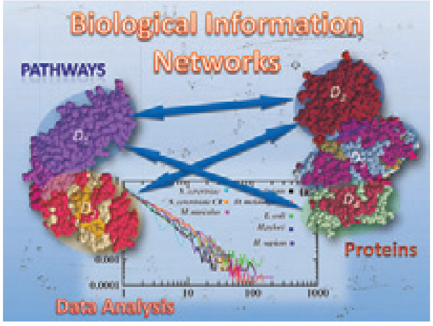
CHEN, Xi The University of Hong Kong, China, P. R., 2 June–13 August

Scope of Research

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

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



Selected Publications

Akutsu T, Fukagawa D, Takasu A, Tamura T: Exact Algorithms for Computing Tree Edit Distance between Unordered Trees, *Theoretical Computer Science*, **421,** 352-364 (2011).
Hayashida M, Akutsu T: Comparing Biological Networks via Graph Compression, *BMC Systems Biology*, **4 (Suppl. 2),** S13 (2010).
Kato Y, Sato K, Hamada M, Watanabe Y, Asai K, Akutsu T: RactIP: Fast and Accurate Prediction of RNA-RNA Interaction Using Integer Programming, *Bioinformatics*, **26,** i460-i466 (2010).
Akutsu T: A Bisection Algorithm for Grammar-Based Compression of Ordered Trees, *Information Processing Letters*, **110,** 815-820 (2010).
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).

Conditional Random Field Approach to Prediction of Protein-Protein Interactions Using Domain Information

Exploration of functions and interactions of proteins and domains is important for understanding cellular systems and biological networks. Many methods for predicting protein-protein interactions have been developed. It is known that mutual information between residues at interacting sites can be higher than that at non-interacting sites. It is based on the thought that amino acid residues at interacting sites have coevolved with those at the corresponding residues in the partner proteins. Several studies have shown that such mutual information is useful for identifying contact residues in interacting proteins.

We propose novel methods using conditional random fields for predicting protein-protein interactions. We focus on the mutual information (MI) between residues, and combine it with conditional random fields. In the methods, protein-protein interactions are modeled using domain-domain interactions. Therefore, MI is calculated for each domain pair as the maximum of MIs between residues.

We perform computational experiments using protein-protein interaction datasets for several organisms, and calculate AUC (Area Under the Curve) score. The results suggest that our proposed methods with and without mutual information outperform EM (Expectation Maximization) method proposed by Deng et al., which is one of the best predictors based on domain-domain interactions. Our methods based on domain-domain interactions are useful for predicting protein-protein interactions.

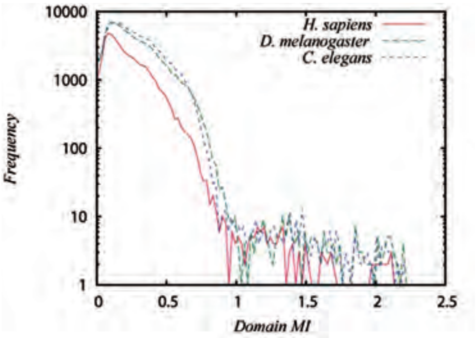


Figure 1. Distributions of domain MIs for *H. sapiens, D. melanogaster,* and *C. elegans*.

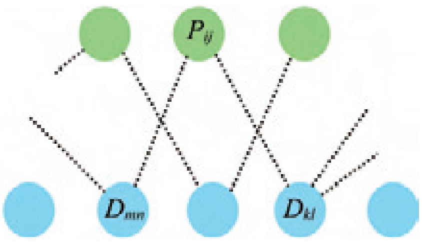


Figure 2. Markov random field model for protein-protein interactions.

Compound Analysis via Graph Kernels Incorporating Chirality

In chemoinformatics and bioinformatics, drug design is one of the main practical and industrial targets. In the development of new pharmaceuticals, in order to find lead compounds, researchers must often select a small subset of compounds from a vastly larger set that satisfies design requirements. After compound selection, high-throughput screening is a method for the synthesis and evaluation of compounds, although it requires considerable time and cost. Therefore, it is advantageous to reduce screening to only those candidates which have been filtered by computational prediction. A major approach to property prediction is to quantitatively analyze the structural features of a compound and find a connection between the target property and features analyzed. This methodology is known as a Quantitative Structure-Activity/Property Relationship (QSAR or QSPR).

In QSPRs, it is very important to achieve high accuracy. Though existing graph-theoretic kernel methods combined with machine learning techniques are efficient for QSPR model construction, they cannot distinguish topologically identical chiral compounds which often exhibit different biological characteristics. In this study, we propose a new method that extends the recently developed tree pattern graph kernel to accommodate stereoisomers. We show that Support Vector Regression (SVR) with a chiral graph kernel is useful for target property prediction by demonstrating its application to a set of human vitamin D receptor ligands currently under consideration for their potential anti-cancer effects.

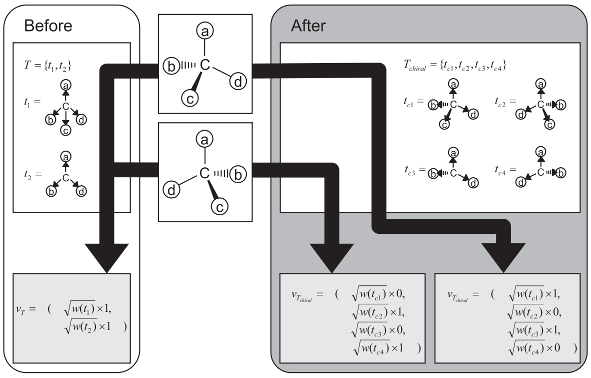


Figure 3. Difference in feature vectors yielded by chirality. Atoms are corresponding to labeled graph nodes, and a bond is corresponding to two oppositely directed graph edges with identical labels indicating the bond order.

Bioinformatics Center
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(D Agr)


PD
HANCOCK, Timothy Peter
(Ph D)

Student

du VERLE, David (D2)

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Assist Prof WICKER, Nicolas	University of Strasbourg, France, 27 February–13 March
Assoc Prof SJOLANDER, Kimmen	University of California, Berkeley, USA, 13 July
Assoc Prof ZHU, Shanfeng	Fudan University, China, P. R., 6–19 June
Prof KNAPP, Ernst-Walter	Free University of Berlin, Germany, 23 July
Prof KRAMER, Stefan	Technical University of Munich, Germany, 25–29 July
Senior Lect LAWRENCE, Neil	University of Manchester, UK, 25–29 July
Assoc Prof XING, Poe	Carnegie Mellon University, USA, 26–29 July
Assoc Prof ESKIN, Eleazar	University of California, Los Angeles, USA, 25–29 July
Dr LANDSMAN, David	National Institute of Health, USA, 25–27 July
Prof SHARAN, Roded	Tel-Aviv University, Israel, 26–29 July
Assoc Prof ZHU, Shanfeng	Fudan University, China, P. R., 24–30 July
Dr BAIROCH, Amos	Swiss Institute of Bioinformatics (SIB), Switzerland, 8 October
Dr LANE, Lydie	Swiss Institute of Bioinformatics (SIB), Switzerland, 8 October
Prof VARNEK, Alexandre	University of Strasbourg, France, 28 October
Assoc Prof LI Jiuyong	University of South Australia, Australia, 2, 9 December

Scope of Research

Mechanisms of biological functions can be shown by pathways in biological networks, such as metabolic network, signal transduction pathways and protein-protein interactions. We are interested in mining pathways related with biological conditions, such as patients/normal, by not only using biological networks but also the data of showing genes/proteins activities such as gene expression. Our approach is to develop new machine learning/data mining techniques for our interest, especially focusing on integrating different types of biological data including networks and graphs in biology.

Selected Publications

Hancock T, Takigawa I, Mamitsuka H: Mining Metabolic Pathways through Gene Expression, *Bioinformatics*, **26 (17),** 2128-2135 (2010).

Hu X, Zhou W, Udaka K, Mamitsuka H, Zhu S: MetaMHC: A Meta Approach to Predict Peptides Binding to MHC Molecules, *Nucleic Acids Research*, **38,** W474-W479 (2010).

Hancock T, Mamitsuka H: Boosted Optimization for Network Classification, *Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS 2010)* (*JMLR: Workshop and Conference Proceedings*), **Vol. 9,** 305-312 (2010).

KEYWORDS

Data Mining
Bioinformatics
Machine Learning
Computational Genomics
Systems Biology

Mining Metabolic Pathways through Gene Expression

Metabolic networks are maps of chemical reaction pathways that are known to occur within a cell. The activity of each metabolic pathway is controlled by the activation and interaction between genetic pathways. For many organisms the reaction structure and genetic dependencies of metabolism have been identified and are stored within the Kyoto Encyclopedia for Genes and Genomes (KEGG) database. The KEGG database reveals that metabolic networks are large and highly complex. This size and complexity is sufficient to hide the key genetic pathways which define the response of the metabolic network to external stimuli.

Pathways of coordinated gene expression determine which metabolic compounds can be synthesized, and thus can define the function of metabolic networks. Additionally, microarray experiments have allowed researchers to measure gene expression under various experimental conditions. Since their inception, bioinformatics methods have tried and combine microarray expression and metabolic networks to identify the pathways that drive an observed response. In this research we have developed a framework to identify the functional metabolic pathways within gene expression.

Our approach is a combination of probabilistic models for pathway ranking, clustering and classification and is freely available as an R package: ***PathRanker***.

PathRanker first employs a non-parametric pathway extraction method to identify the most highly correlated paths through the metabolic network. Figure 1 presents an image the top 1000 pathways for yeast in *stationary phase* compared with control observations. In Figure 1 each row is a pathway and each column is a gene. The left plots show the probability and *p*-value of each path, and the bottom bar plot displays the probability of a gene over all paths. Clearly visible in Figure 1 is a block of pathways defines yeast's stationary phase.

PathRanker can then extract the defining structure within the top ranked pathways using Markov clustering and classification algorithms. The result of 3M Markov clustering is presented in Figure 2. The pathways in Figure 2 summarize 93% of yeast's stationary phase pathways. The analysis of these identified pathways can be performed at multiple resolutions including interacting genes, reactions, compounds and pathways (Figure 2). We also confirm the importance of these pathways from a biological perspective.

Finally we would like to emphasize that integrating probabilistic path ranking with clustering or classification is a reasonable combination in terms of machine learning, because path ranking generates tons of pathways which might be redundant because of the complex nature of metabolic networks while a large number of pathways can be summarized by clustering or classification.

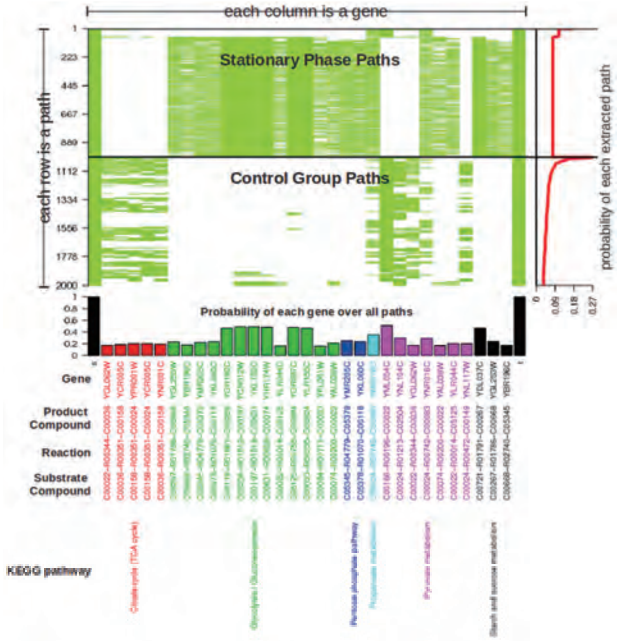

Figure 1.

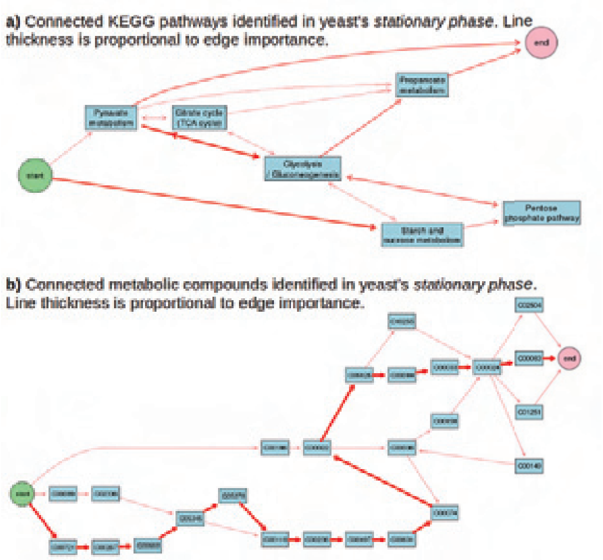

Figure 2.

Endowed Research Section
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Program-Specific Assist Prof
TSUJINO, Yasuo

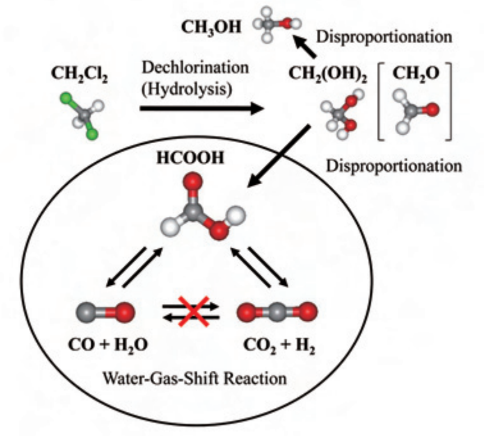
Researcher

ISOBE, Akira

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 does make a contribution to the CO_2 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 CO_2 on a large scale. Fundamental aspects of pyrolysis of ethers (unimolecular reaction of ethers) are also investigated by NMR.

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



Selected Publications

Yasaka Y, Wakai C, Matubayasi N, Nakahara M: Controlling the Equilibrium of Formic Acid with Hydrogen and Carbon Dioxide Using Ionic Liquid, *J. Phys. Chem. A*, **114,** 3510-3515 (2010).

Nakahara M, Tsujino Y, Yoshida K, Yasaka Y, Uosaki Y, Wakai C, Matubayasi N: Recent Advances in Studies on Organic Reactions in Water at High Temperatures and High Pressures, *Rev. High Pressure Sci. Technol*, **20,** 40-49 (2010) (in Japanese).

Yasaka Y, Yoshida K, Wakai C, Matubayasi N, Nakahara M: Kinetics and Equilibrium Study on the Formic Acid Decomposition in Relation to the Water-Gas-Shift Reaction, *J. Phys. Chem. A*, **110,** 11082-11090 (2006).

Matubayasi N, Nakahara M: Hydrothermal Reactions of Small Compounds: Free-energy Analysis of Equilibrium, *J. Chem. Phys.*, **122,** 074509-074520 (2005).

Yoshida K, Matubayasi N, Uosaki Y, Nakahara M: Scaled Polynomial Expression for Self-Diffusion Coefficients for Water, Benzene, and Cyclohexane over a Wide Range of Temperatures and Densities, *J. Chem. Eng. Data*, **55,** 2815-2823 (2010).

Green Chemical Approach to Energy and Environmental Problems Using Hot Water and Carbon Dioxide

Millions of natural and artificial organic and inorganic compounds have been found and synthesized by scientists and made useful directly in a KYOUSEI or earth-friendly style or after the industrial mass production. The materials processing and commercialization have helped us improve our way of life, welfare, and democracy for the past 300 years. Nevertheless molecular and/or ionic systems of tens of atoms, nanometer-sized, are not yet fully understood and utilized in harmony or coexistence with our environment (KYOUSEI). More advances in green science and technology are required for achieving the dream of society sustainability by solving environment and energy resource issues under the conditions of KYOUSEI. We should develop the green chemistry of rather small and simple molecules in hot water in order to reduce CO_2 emission. Thus we need to invent renewable synthetic fuels.

Energy is continuously necessary for keeping or developing our welfare for billions of people on Earth. The world-wide motorization can liberate us from severe labor work for men and women, e.g., coal and gold mining and house-keeping work. However civilization, a departure from the genuinely green primitive life, requires energy. Energy is generated by the oxidation of such fossil fuels as coal, petroleum, and natural gases where solar energy is chemically accumulated through photosynthesis by chlorophylls after the transformation and integration. Chemical energy is used directly in mechanical engines or indirectly through electricity. Also human beings and wild animals eat naturally produced or processed foods for the internal burning to generate energy. Anyway we consume energy and plants or greens on land and in sea storing energy from Sun into the chemical bonds, C-C, C-H, OH, etc. that lead to the exothermic oxidation reactions. Is our civilization merely destined to be like this? Are there no detours? Answers to these questions can create green chemistry. Can chemistry find them? Yes we can. A detour must be green. Such a green chemical way can be constructed by preventing or delaying the fossil burning as much as we can. The burning of hydrogen results only at the production of H_2O that is essentially our Earth environment because our planet is covered with water in the hydrosphere. Change the burning from carbon to hydrogen as much as we can. How to get hydrogen at a *low* cost? Cheap hydrogen is generated in iron works where hydrogen is generated as a by-product from the reaction of supercritical water and carbon, the water-gas-shift reaction. Such by-product hydrogen is also produced on a large scale by electrolysis of aqueous NaCl solution in soda industries.

Toward a new-generation hydrogen-fuel technology, we propose formic acid, which is hydrothermally connected with H_2, CO, and CO_2, as a chemical tank for hydrogen storage and transportation. This is a new version of the industrially famous water-gas-shift reaction.

In sub- and supercritical water, formic acid decomposes without catalysts in the following two pathways:

$$HCOOH \rightleftarrows CO + H_2O \text{ (decarbonylation)} \qquad (1)$$

$$HCOOH \rightleftarrows CO_2 + H_2 \text{ (decarboxylation)} \qquad (2)$$

The reversibility of the decarbonylation has been discovered by the direct NMR observation of the conversion of CO to HCOOH in hot water and furthermore by the stability analysis based on the free energies for the simple molecules (HCOOH, CO, CO_2, H_2, and H_2O) involved. The reversibility and the coupling of the reactions given by reactions (1) and (2) clearly indicate that formic acid exists as an intermediate in the water-gas-shift (WGS) reaction, which has long been known to generate hydrogen from water as a clean fuel. Now the new expression of the WGS reaction is:

$$CO + H_2O \rightleftarrows HCOOH \rightleftarrows CO_2 + H_2 \qquad (3)$$

The kinetics and equilibrium of the new WGS reaction can be comprehensively established by determining the rate and equilibrium constants for the decarbonylation and the decarboxylation of formic acid by means of NMR. The kinetic and equilibrium investigations are carried out on the hydrothermal decomposition processes (1) and (2) of formic acid, the intermediate of the water-gas-shift (WGS) reaction, in hot water at temperatures of 170-330 °C. On the basis of the kinetics and equilibrium of the formic acid decomposition, the WGS reaction (3) can be controlled in a desirable direction by tuning temperature and pH of hot water. To develop the concept of the chemical-tank HCOOH for H_2 the optimization of the reaction parameters, such as temperature, pressure, and solvent (room temperature ionic liquids) is intensively surveyed. It has been found that when the temperature lowered to 150 °C the yield of HCOOH increases by a factor of 500 despite the slowdown of the reaction rate. The formation of HCOOH is exothermic as predicted.

[Adapted from the key-note lecture by M. Nakahara in the International, 10th KYOUSEI Science Center Symposium, Nara Women's University, 4 December 2010.]

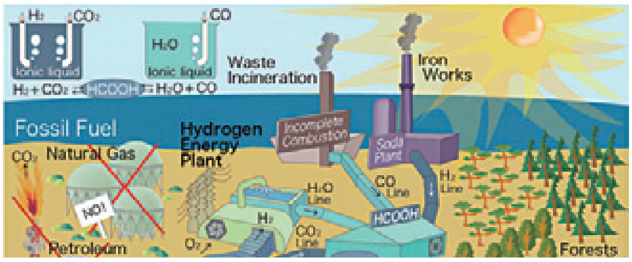


Figure 1. The hydrogen-water-energy-cycle via formic acid intermediate by using the water-gas-shift reaction.

JURC COOPERATIVE RESEARCH SUBJECTS

JURC COOPERATIVE RESEARCH SUBJECTS

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

Measurement of Electron Density by Compton Scattering CT
YAMAZAKI, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC NODA, Akira

Development and Apprication of Time-resolved Irradiation Method by Cooled Ion Beams
NODA, Koji, National Institute of Radiological Sciences
Host in JURC NODA, Akira

X-ray Structural Studies on Cold Adaptation of Protein from Psychrophile
GOGAMI, Yoshitaka, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in JURC HATA, Yasuo

Synthesis of Metal-Containing Phenolic Resins toward Optical Material with High Refractive Index
KONISHI, Gen-ichi, Faculty of Science and Technology, Tokyo Institute of Technology
Host in JURC OZAWA, Fumiyuki

Investigations of the Ground State and Magnetic Excitations in Frustrated Magnets
KIKUTCHI, Hikomitsu, Faculty of Enginnering, University of Fukui
Host in JURC AZUMA, Masaki

Mechanistic Study and Development of Iron-Catalyzed C–C Bond Forming Reactions
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC NAKAMURA, Masaharu

Extraction Behavior of Metal Ions in Liquid-liquid Extraction Using Novel Multidentate Ligands
MUKAI, Hiroshi, Kyoto University of Education
Host in JURC SOHRIN, Yoshiki

Facile Synthesis of Alkynyl Sugars by Iron-Catalyzed Cross-Coupling Reaction and Its Application to Stimuli-Responsive Luminescence
ORITA, Akihiro, Faculty of Engineering, Okayama University of Science
Host in JURC NAKAMURA, Masaharu

Rice Metabolic Pathway Construction from Highly Accurate Rice Annotation
ITOH, Takeshi, National Institute of Agrobiological Sciences
Host in JURC GOTO, Susumu

Aphid Pathway Reconstruction from Genome Information
SHIGENOBU, Shuji, National Institute for Basic Biology
Host in JURC KANEHISA, Minoru

Efficient and Flexible Algorithms for Pattern Matching of Tree-structured Data in Bioinformatics
TAKASU, Atsuhiro, National Institute of Informatics
Host in JURC AKUTSU, Tatsuya

Repetition Structure Analysis of Genome Sequences Based on Global Evaluation Measures
NAKAMURA, Atsuyoshi, Graduate School of Information Science and Technology, Hokkaido University
Host in JURC MAMITSUKA, Hiroshi

Cornea Regeneration by Cell-adhesion-promoting Small Molecules
KOIZUMI, Noriko, Faculty of Life and Medical Sciences, Doshisha University
Host in JURC UESUGI, Motonari

Study on the Fabrication Process of Organic-inorganic Hybrid Materials
FUJINO, Shigeru, Graduate School of Engineering, Kyushu University
Host in JURC YOKO, Toshinobu

Development of New Boryl Groups to Create Water-Soluble Highly Emissive π-Electron Materials
FUKAZAWA, Aiko, Department of Chemistry, Graduate School of Science, Nagoya University
Host in JURC MURATA, Yasujiro

Transdermal Drug Delivery Using Arginine-rich Peptides
KOGURE, Kentaro, Kyoto Pharmaceutical University
Host in JURC FUTAKI, Shiroh

Modulation of Spin-Wave Dispersion in Heterostructures
YAMAGUCHI, Akinobu, Department of Physics, Keio University
Host in JURC ONO, Teruo

Correlation of Structure and Electronic Structure in Thin Films of Group 10 Metals Dione-Dioximato
TAKEDA, Keiki, Muroran Institute of Technology
Host in JURC SATO, Naoki

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

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

Multi-dimensional Doppler Laser Cooling for Realization of Ultralow-temperature Ion Beam
ITO, Kiyokazu, Graduate School of Advanced Sciences of Matter, Hiroshima University
Host in JURC NODA, Akira

Development and Mechanism Investigation of Non-Planar Carbocations on a Redox Active Tetrairon Cores
OKAZAKI, Masaaki, Faculty of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Study of the Localization Mechanism and the Optical Properties in the Wide Band-gap GaN-based Semiconductors
YAMADA, Yoichi, Department of Electrical and Electronic Enginnering, Yamaguchi University
Host in JURC KANEMITSU, Yoshihiko

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

Effective Intracellular siRNA Delivery Using PNA-CPP Conjugates
KITAMATSU, Mizuki, Graduate School of Natural Science and Technology, Okayama University
Host in JURC FUTAKI, Shiroh

Comprehensive Analysis of Proteolytic Modulation by the Integrated Data-mining Method
SORIMACHI, Hiroyuki, The Tokyo Metropolitan Institute of Medical Science
Host in JURC MAMITSUKA, Hiroshi

Development of Functional Prediction Method of Cytochrome 450s Involved in Steroid Hormone Biosynthesis and Metabolism
OONISHI, Toshiyuki, Global Institute for Young Scientists of Shizuoka University
Host in JURC WATANABE, Bunta

Development of Novel Solid-type Polyelectrolyte Membrane by Living Radical Polymerization
SATO, Takaya, Tsuruoka National College of Technology
Host in JURC TSUJII, Yoshinobu

Synthesis and Characterization of Concentrated Polymer Brushes with Glucose-sensing Ability
YOSHIKAWA, Chiaki, National Instuituite for Materials Science
Host in JURC TSUJII, Yoshinobu

Structure Engineering and Function Controlling of Hollow Fibers for Biophotonics
SHIOTA, Yoshihito, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC TOKUDA, Yomei

Coupled Quantum-Chemical and Statistical-Mechanical Analysis of Biochemical Reactions
TAKAHASHI, Hideaki, Graduate School of Science, Tohoku University
Host in JURC MATUBAYASI, Nobuyuki

Structure of Frustrated Polymer Crystal at Extremely Low Temperature
OKIHARA, Takumi, Graduate School of Natural Science and Technology, Okayama University
Host in JURC TSUJI, Masaki

Dynamical Inhomogeneity in Miscible Polymer Blends
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Precise Structure Control of Polymer by Using External Fields
ITO, Hiroshi, Faculty of Science and Engineering, Yamagata University
Host in JURC KANAYA, Toshiji

Studies on Crystal Structure and Crystallization of Polylactic Acid
KAWAI, Takahiko, Faculty of Engineering, Gunma University
Host in JURC KANAYA, Toshiji

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

Study on the Tunneling Magnetoresistance and Local Magnetism in Magnetic Tunnel Junction Devices with Ferromagnetic Electrodes of Heusler Alloy Co_2MnSn Made by Atomic Layer Deposition
TANAKA, Masaaki, Department of Electrical and Electronic Engineering, Nagoya Institute Technology
Host in JURC ONO, Teruo

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

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

THz Generation by Laser-cluster Interactions
NAGASHIMA, Takeshi, ILE, Osaka University
Host in JURC SAKABE, Shuji

Supramolecular Multi-Metal Catalyst for Selective Degradaton of Lignin
WATANABE, Takashi, Research Institute for Sustainable Humanoshere, Kyoto University
Host in JURC NAKAMURA, Masaharu

Silicon Photonics in the Novel Silicon Sulfide Phosphors
OKUNO, Tsuyoshi, Department of Applied Physics and Chemistry, The University of Electro-Communications
Host in JURC KANEMITSU, Yoshihiko

Synthesis and Properties of Crosslinked Oligonaphthalenes
KURAMOCHI, Koji, Graduate School of Life and Environmental Science, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo

Exploring New Electronic Properties by the Electronic State Control in Semiconductor Using Nano Magnets
HASHISAKA, Masayuki, Research Center for Low Temperature Physics, Tokyo Institute of Technology
Host in JURC KOBAYASHI, Kensuke

Overproduction of Milaculin in *Arabidopsis thaliana*
INOUE, Hiroyasu, Faculty of Human Life and Environment, Nara Women's University
Host in JURC AOYAMA, Takashi

Structural Analysis of Protein Complex through Hierachical Modelling Flow with Bioinformatics, Large-Scale Molecular Simulation, and Solution Theory
KITAO, Akio, Institute of Molecular and Cellular Biosciences, The University of Tokyo
Host in JURC MATUBAYASI, Nobuyuki

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

High-energy Ion Generation by Laser Nano-particle Interactions
NAKAI, Mitsuo, ILE, Osaka University
Host in JURC SAKABE, Shuji

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

Extensional Rheology of Polymers
NISHIOKA, Akihiro, Faculty of Engineering, Yamagata University
Host in JURC WATANABE, Hiroshi

Study of the Regulatory Mechanism for Cell Differentiation in Epidermal Cells of Higher Plants
TAKAHASHI, Taku, Graduate School of Natural Science and Technology, Okayama University
Host in JURC AOYAMA, Takashi

Hydration Dynamics of Functional, Multivalent Ions
SUZUKI, Makoto, Graduate School of Engineering, Tohoku University
Host in JURC MATUBAYASI, Nobuyuki

Dynamics of Supramolecules
SHIKATA, Toshiyuki, Graduate School of Science, Osaka University
Host in JURC MASUBUCHI, Yuichi

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Construction of a Library of Heterocyclic Compounds with Tetrasubstituted Carbon and Search for Biologically Active Compounds
ISHIBASHI, Masami, Graduate School of Pharmaceutical Sciences, Chiba University
Host in JURC KAWABATA, Takeo

Development of Induction System Using Caged Chemical in Plants
NOZAKI, Hiroshi, the Faculty of Science, Okayama University of Science
Host in JURC AOYAMA, Takashi

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

Explorations of Novel Electronic Phases in Iron-titanium Hybrid Materials with Various Atomic Valence States
FUJII, Tatsuo, Faculty of Engineering, Okayama University
Host in JURC SHIMAKAWA, Yuichi

Generation of Highly Reactive Species by Chemical Reaction inside Fullerenes
AKASAKA, Takeshi, Life Science Center of Tsukuba Advanced Research Alliance, University of Tsukuba
Host in JURC MURATA, Yasujiro

Function of a Novel Multiheme Selenoprotein from a Metal-reducing Bacterium, *Geobacter sulfurreducens*
MIHARA, Hisaaki, College of Life Sciences, Ritsumeikan University
Host in JURC KURIHARA, Tatsuo

Development of High Performance Nanofibers from Silk Fibroin
KAWAHARA, Yutaka, Faculty of Engineering, Gunma University
Host in JURC TSUJI, Masaki

Photochemical Properties of Poly(phenylenevinylene)s
IKEGAMI, Masashi, Graduate School of Engineering, Toin University of Yokohama
Host in JURC OZAWA, Fumiyuki

SUBJECTS FOCUSING ON JOINT USAGE OF JURC/ICR FACILITIES

Solvent Effect for Structure and Reactivity of Diacetylene Molecular Film
TAKAJO, Daisuke, School of Science, Osaka University
Host in JURC KURATA, Hiroki

Degradation of Optical Properties in First Mirror Materials for Plasma Diagnostics by Nano-EELS
ONO, Kotaro, Interdisciplinary Faculty of Science and Engineering, Shimane University
Host in JURC KURATA, Hiroki

Solid-State NMR Analysis of Molecular Orientation in Organic LED Materials
YAHIRO, Masayuki, Center for Future Chemistry, Kyusyu University
Host in JURC KAJI, Hironori

Photocatalytic Degradation of Acetaldehyde on WO3 Film Surface: Solid-State NMR Study on Reactive Mechanism
SHIGESATO, Yuzo, Graduate School of Science and Engneering, Aoyama Gakuin University
Host in JURC KAJI, Hironori

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

Synthesis of Transition Metal Complexes Bearing Novel Tetradantate Tripodal Ligands and Their Structural Characterization
UNNO, Masafumi, Graduate School of Engineering, Gunma University
Host in JURC TOKITOH, Norihiro

Elucidation of the Physical and Chemical Properties of Novel Aromatic Compounds Containing Heavier Group 14 Elements
SAITO, Masaichi, Graduate School of Science and Engineering, Saitama University
Host in JURC TOKITOH, Norihiro

SUBJECTS ENCOURAGING JOINT PROGRAM

Electronic States and Local Structures in Transition Metal Oxide Thin Films Probed by Sybchrotron Xray
MIZUMAKI, Masaichiro, Japan Synchrotron Radiation Research Institute
Host in JURC SHIMAKAWA, Yuichi

The International Workshop for East Asian Young Rheologists
SAKURAI, Shin-ichi, Graduate School of Biobased Materials Science, Kyoto Institue of Technology
Host in JURC WATANABE, Hiroshi

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
FUJIWARA, Takumi
(D Eng)

Laboratory of Inorganic Photonics Materials

Professor, Graduate School of Engineering, Tohoku University
(Aramaki, Aoba-ku, Sendai 980-0845)

Lectures at *ICR*
Micro-optical Functional Glasses Prepared by Laser-processing

Vis Prof
ADACHI, Chihaya
(D Eng)

Laboratory of Molecular Materials Chemistry

Professor, Center for Future Chemistry, Kyusyu University
(744 Motooka, Nishi, Fukuoka 819-0395)

Lectures at *ICR*
Novel Organic Light Emitting Diodes Using Delayed Fluorescence and Molecular Orientation

Vis Prof
AWAZU, Kunio
(D Eng and D Med)

Laboratory of Laser Matter Interaction Science

Professor, Graduate School of Enginerring, Osaka University
(2-3 Yamadaoka, Suita Osaka, 565 Japan)

Lectures at *ICR*
The Present and the Future of Laser Medical Treatment –Toward the Disease-selective Laser Medical Treatment–

Vis Prof
ASAI, Kiyoshi
(D Eng)

Laboratory of Pathway Engineering

Professor, Department of Computational Biology, The University of Tokyo
(5-1-5 Kashiwanoha, Kashiwa-shi, Chiba-ken 277-8561)

Lectures at *ICR*
On Development of the Techniques for Analyzing RNA Sequence Information

Vis Prof
SOLOSHONOK, Vadim A.
(Ph D)

Laboratory of Organotransition Metal Chemistry

Professor, Department of Chemistry and Biochemistry, The University of Oklahoma
(620 Parrington Oval, Room 208, Norman, Oklahoma 73019-3051, USA)

Research Subject at *ICR*
Development of Theory and Nomenclature for Chirial Nano-tube

Vis Prof
SHING, Tony K M
(Ph D)

Laboratory of Organic Main Group Chemistry

Professor, Department of Chemistry, The Chinese University of Hong Kong
(Hong Kong, China, P.R.)

Lectures at *ICR*
Carbocyclization of Carbohydrates: Syntheses of Bioactive Hydroxylated Cycloalka(e)nes–Calistegines, Gabosines and Pseudo-Acarviosin

Vis Prof
KENNEDY, Brendan J.
(Ph D)

Laboratory of Advanced Solid State Chemistry

Professor, School of Chemistry, University of Sydney
(School of Chemistry, Building F11 The University of Sydney, NSW, 2006, Australia)

Lectures at *ICR*
Structure and Magnetism in a Technetium Oxide

Vis Assoc Prof
ARAI, A. Midori
(D Pharm Sc)

Laboratory of Synthetic Organic Chemistry

Associate Professor, Graduate School of Pharmaceutical Sciences, Chiba University
(1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan)

Lectures at *ICR*
Approaches to Neural Stem Cells or Cancer Cells Based on Natural Products

Vis Assoc Prof
HAYASHI, Ken-ichiro
(D Agr)

Laboratory of Molecular Biology

Associate Professor, Natural Product Chemistry Laboratory, Okayama University of Science
(1-1, Ridai-cho, Okayama 700-0005)

Lectures at *ICR*
Chemical Biology of the Phytohormone Auxin

Vis Assoc Prof
MATSUBA, Go
(D Eng)

Laboratory of Polymer Materials Science

Associate Professor, Faculty of Science and Engineering, Yamagata University
(4-3-16 Jonan, Yonezawa, Yamagata 992-8510)

Lectures at *ICR*
Function Control through the Analysis of Polymer Crystallization Process

Vis Assoc Prof
HAYASHI, Katsuro
(D Eng)

Laboratory of Advanced Solid State Chemistry

Associate Professor, Secure Materials Research Center , Tokyo Institute of Technology
(4259 Nagatsuta, Midori-ku, Yokohama 226-8503)

Lectures at *ICR*
Mayenite as a Functional Transparent Oxide

PERSONAL

Awards

TOKITOH, Norihiro

The 3rd Kim Yong Hae Lectureship Award

KAIST, Korea

1 September 2010

Award for the Best Reviewers of Grant-in-Aid for Scientific Research

Japan Society for the Promotion of Science

29 October 2010

SASAMORI, Takahiro

The Chemical Society of Japan Award for Young Chemists for 2009

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

The Chemical Society of Japan

27 March 2010

MIZUHATA, Yoshiyuki

ICR Award for Young Scientists

“1,2-Dialkynyldisilenes: Silicon Analogues of (*E*)-Enediyne”

Institute for Chemical Research, Kyoto University

10 December 2010

TANABE, Yusuke

The Best Oral Presentation Award

The 90th Annual Meeting of the Chemical Society, Japan

“Synthesis, Structure, and Properties of a Silicon Analogue of Biphenyl”

The Chemical Society of Japan

14 April 2010

FURUTA, Takumi

Takasago Koryo Kogyo Award in Synthetic Organic Chemistry, Japan

“Development of Molecular Recognizable Biaryl Catalysts for Efficient Synthesis of Bioactive Polyols”

The Society of Synthetic Organic Chemistry, Japan

19 February 2010

YAMAGO, Shigeru

The Chemical Society of Japan Award for Creative Work

“Development of Precision Radical Reactions Exploiting Reactivities of Heteroatom Compounds”

The Chemical Society of Japan

27 March 2010

Asian Core Program Lectureship Award

The 1st New Phase Asian Core Program on Cutting-Edge Organic Chemistry in Asia

“Synthesis of Cycloparaphenylenes from Square-Shaped Tetranuclear Platinum Complexes”

The New Phase Asian Core Program on Cutting-Edge Organic Chemistry in Asia (Singapore)

10 November 2010

KAYAHARA, Eiichi

CSJ Student Presentation Award 2010

The 90th Annual Meeting of the Chemical Society of Japan

“Theoretical Studies of Heteroatomic Effect on Homolytic Substitution Reaction of Group 15, 16 and 17 Diheteroatom Compounds with Carbon-Centered Radicals”

The Chemical Society of Japan

14 April 2010

MASAI, Hirokazu

The Best Oral Presentation Award

The 71st Autumn Meeting, 2010, the Japan Society of Applied Physics

“Emission Property of Sn-doped Phosphate Glass and the Optical Application”

The Japan Society of Applied Physics

14 September 2010

NAKAMURA, Shuji

ICR Award for Graduate Students

“Nonequilibrium Fluctuation Relations in a Quantum Coherent Conductor”

Institute for Chemical Research, Kyoto University

10 December 2010

SUZUKI, Furitsu

The Encouragement Award for Young Scientist

The 9th General Meeting of Japan Society of Organic Electroluminescence Devices

“Charge Transfer Rate Constants and Charge Transfer Paths of Hole- and Bipolar-Transport Organic Materials, TPD and CBP, Based on Marcus Theory”

Japan Society of Organic Electroluminescence Devices

17 June 2010

AMR, Mohammed Hassan

Best Presentation Award

The 57th Annual Conference of the Japanese Biochemical Society, Kinki Branch

“Mechanism of 2-haloacrylate Hydratase Reaction: Evidence for the Involvement of a Radical Chemistry in the Hydration of 2-chloroacrylate”

The Japanese Biochemical Society, Kinki Branch

22 May 2010

HASHIMOTO, Toru

ICR Award for Graduate Students

“Iron-Catalyzed Suzuki-Miyaura Coupling of Alkyl Halides”

Institute for Chemical Research, Kyoto University

10 December 2010

NAKAMURA, Yoshitaka

The Incentive Award for Excellent Presentation

The 57th Spring Meeting of the Japan Society of Applied Physics

“Preparation and Characterization of (1-x)$BiFeO_3$-x$BiCoO_3$ Thin Films with a Large Tetragonal Distortion”

The Japan Society of Applied Physics

14 September 2010

KANEMITSU, Yoshihiko

Outstanding Achievement Award of the 125th Research Committee on Mutual Conversion between Light and Electricity

Japan Society for Promotion of Science

25 October 2010

Paper Awards

TSURUSAKI, Akihiro; NAGAHORA, Noriyoshi; SASAMORI, Takahiro; MATSUDA, Kazunari; KANEMITSU, Yoshihiko; WATANABE, Yasuaki[1]; HOSOI, Yoshinobu[1]; FURUKAWA, Yukio[1]; TOKITOH, Norihiro

BCSJ Award

“Synthesis, Structures, and Reactivity of Kinetically Stabilized Anthryldiphosphene Derivatives”

The Chemical Society of Japan

15 March 2010

1. Department of Chemistry & Biochemistry, School of Advanced Science and Engineering, Waseda University

NAKAMURA, Shuji

IUPAP Young Author Best Paper Awards

The 30th International Conference on the Physics of Semiconductors (ICPS 2010)

“Nonequilibrium Fluctuation Relations in a Quantum Coherent Conductor”

The International Union of Pure and Applied Physics (IUPAP)

30 July 2010

MASUBUCHI, Yuichi

The Best Paper Award 2010

“Primitive Chain Network Simulations of Conformational Relaxation for Individual Molecules in the Entangles State”

The Society of Rheology, Japan

13 May 2010

HAYES, Nelson; DEIZ, Diego; JOANNIN, Nicolas[1,2]; KANEHISA, Minoru; WAHLGREN, Mats[1,2]; WHEELOCK, Craig E.[3]; GOTO, Susumu

GIW2009 Best Paper Awards

GIW2009: The 20th International Conference on Genome Informatics

“Tools for Investigating Mechanisms of Antigenic Variation: New Extensions to varDB”

International Conference on Genome Informatics

16 December 2009

1. Department of Microbiology, Tumor and Cell Biology, Karolinska Institutet, Sweden
2. Swedish Institute for Infectious Disease Control (Smittskyddsinstitutet), Sweden
3. Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Sweden

Poster Awards

MIZUHATA, Yoshiyuki

Best Poster Award

The 13th International Conference on the Coordination and Organometallic Chemistry of Germanium, Tin, and Lead

“Generation and Properties of Stannabenzenes”

Organizing Committee of ICCOC-GTL-13

15 July 2010

MIEDA, Eiko

The Best Poster Award

The 37th Symposium on Main Group Element Chemistry “Studies on the Generation of a Fluorosilene Bearing Bulky Substituents”

Organizing Committee of the 37th Symposium on Main Group Element Chemistry

27 November 2010

SUGAMATA, Koh

The Best Poster Award

The 36th Symposium on Main Group Element Chemistry

“Synthetic Studies on Stable Cation Species of Dichalcogenides”

Organizing Committee of the 36th Symposium on Main Group Element Chemistry

12 December 2009

MORINAKA, Yuta

Poster Award

42th Symposium on Structural Organic Chemistry for Young Scientists

“Transformation of the Cage-opened Fullerene Derivative with Grignard Reagents”

The Society of Structural Organic Chemistry for Young Scientists

8 August 2010

Young Scientist Poster Award

The 39th Fullerene Nanotubes General Symposium

“Tuning of LUMO levels of Cage-Opened C_{60} Derivatives and Performance of Organic Photovoltaic Devices”

The Fullerene and Nanotubes Research Society

4 October 2010

YOSHIDA, Keisuke

Best Poster Award

40th Congress of Heterocyclic Chemistry

“Regioselective Acylation of 2-amino-1,5-pentanediols by PPY Catalysts with Functional Side Chains”

Organizing Committee of 40th Congress of Heterocyclic Chemistry

16 October 2010

WATANABE, Kazuya

The Poster Award for Young Scientists

The 59th Annual Meeting of the Japan Society for Analytical Chemistry

“Metal Ion Adsorption Behaviors with Molecularly Imprinted Silica Gel Sorbents Having Amino Ligands”

The Japan Society for Analytical Chemistry

15 September 2010

ASAKAWA, Harutoshi

Award for Best Poster Presentation

Future Trends in Softmaterial Research with Advanced Light Source: Interdisciplinary of Bio- & Synthetic-Materials and Industrial Transfers, Japan

“Crystallization of Isotactic Polypropylene from Mesomorphic Phase –A Constant Heating Rate Study–”

JST ERATO and CREST, Japan

3 September 2010

HIRAMOTO, Keisuke

The Best Presentation Award

The 2010 Annual Meeting of the Society of Rheology, Japan

“Component Dynamics in Polyisoprene and Poly(4-tert-butylstyrene) Miscible Blends: A Study of Local Heterogeneity”

The Society of Rheology, Japan

13 May 2009

KAWASAKI, Yohji

The Best Presentation Award

The 2010 Autumn Meeting of the Society of Rheology, Japan

“Blending Law for the Entanglement Length and Local Dynamics in PI/PtBS Miscible Blend”

The Society of Rheology, Japan

5 October 2010

ITOH, Takuma

Award for Distinguished Student Poster

The 6th International Symposium on Integrated Synthesis (ISIS-6)

“Diastereoselective Carbozincation of Oxa- and Azabicyclic Alkenes under Iron Catalysis”

Organizing Committee of ISIS-6

24 October 2010

OKADA, Yoshihiro

Best Poster Award

57th Symposium on Organometallic Chemistry, Japan

“Iron-Catalyzed Cross-Coupling of Alkyl Halides with Alkynylmagnesium Reagents”

The Kinki Chemical Society, Japan

10 December 2010

ICHIKAWA, Noriya

Symposium N (Functional Oxide Nanostructures and Heterostructures) 2010 1st Poster Prize

Materials Research Society Spring Meeting (San Francisco, CA, USA)

“Low-temperature Reduction and Oxidation of $SrCoO_{2.5}$ Thin Films”

Materials Research Society, USA

8 April 2010

MATSUNAGA, Ryusuke

The 37th Fullerene Nanotubes General Symposium Young Scientist Poster Award

The 37th Fullerene Nanotubes General Symposium

“Origin of the Satellite Photoluminescence Peaks in Single SWNTs”

The Fullerenes and Nanotubes Research Society

3 March 2010

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

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ENDOWED RESEARCH SECTION
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Tsinghua University

University of Science and Technology of China, Department of Modern Mechanics

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Institut Laue-Langevin

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Max Planck Institute for Mathematics in the Sciences

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Brown University, Department of Chemistry

Columbia University, Department of Chemistry

Columbia University, Department of Physics

Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory, Materials Sciences Division and Environmental Energy Technologies Division

Rice University, Department of Chemistry and Bioengineering

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

University of California, Department of Chemical Engineering

University of California, Santa Barbara, Materials Department

University of Florida, Department of Chemistry

University of Hawaii, Department of Oceanography

Yale University, Department of Physics

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

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

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

Sasamori T, Construction of 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.

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

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

Kawashima T, Kobayashi J, Agou T, Development of Dimensionally-Extended Hetero-π-conjugated Molecules, Grant-in-Aid for Scientific Research (B), 1 April 2009–31 March 2012.

— Structural Organic Chemistry —

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

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

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

Wakamiya A, Development of Organic Dyes Based on Fine Tuning of π-Orbitals Using DFT Calculations, PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency, 1 October 2010–31 March 2016.

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

— Synthetic Organic Chemistry —

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

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, Asymmetric Total Syntheses of Bioactive Natural Products via Planar Chiral Enolates, Grant-in-Aid for Young Scientists (B), 1 April 2009–31 March 2011.

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

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

Tsujii Y, Development of Novel Nanosystems by Hierarchically Assembling Concentrated Polymer Brushes, CREST Program by JST, 1 October 2009– 31 March 2012.

Tsujii Y, Research and Development of Safe Solid-Electrolyte by Hybridization of Ionic Liquids and Polymers, Research and Development for Promotion of Regional Innovation Program by JST, 9 August 2010–31 March 2011.

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

— Polymer Controlled Synthesis —

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

— Inorganic Photonics Materials —

Masai H, Fabrication of Glass-ceramic Containing Oxide Semiconductor and Metal Nanocrystallites, Grant-in-Aid for Young Scientists (B), 1 April 2010 –31 March 2013.

Masai H, Fabrication of White Phosphor for UV LED Using Low-melting Glass, Adaptable and Seamless Technology Transfer Program through Target-driven R&D, 1 October 2010 –31 March 2011.

— Nanospintronics —

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

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

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

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki S, Novel Methods for Delivering Nucleic Acids Therapeutics, JST, Strategic Japanese-Swedish Cooperative Programme on "Multidisciplinary BIO", 1 July 2009–30 June 2012.

— Chemistry of Molecular Biocatalysts —

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

— Molecular Biology —

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

Tsuge T, Regulatory Mechanism of Plant Morphogenesis by the Regulator of mRNA Metabolism SAP130, Grant-in-Aid for Scientific Research (C), 1 April 2010–31 March 2012.

— Chemical Biology —

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, 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.

DIVISION OF ENVIRONMENTAL CHEMISTRY

—Molecular Materials Chemistry—

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

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

Goto A, Fundamentals and Applications of New Living Radical Polymerization, Kyoto University Step-up Research Grant, 4 June 2009–31 March 2010.

—Hydrospheric Environment Analytical Chemistry—

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

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

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

—Solution and Interface Chemistry—

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

—Molecular Microbial Science—

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

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

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

Kurihara T, Construction of a New Protein Expression System by Using Cold-Adapted Microorganisms Isolated from Polar Regions, Research Grant from Institute for Fermentation, Osaka (IFO), 1 April 2010–31 March 2011.

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

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
—Polymer Materials Science—

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.

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

—Molecular Rheology—

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

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

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

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

Matsumiya Y, Analysis on Mechanical Properties of Multi-Component Fluids Utilizing Dielectric Measurements, Grant-in-Aid for Young Scientists Research (B), 1 April 2010–31 March 2012.

Uneyama T, Theory of Mechanical and Dielectric Response of Polymers under Shear Flow, Grant-in-Aid for Young Scientists (B), 1 April 2010–31 March 2012.

—Molecular Aggregation Analysis—

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.

—Supramolecular Biology—

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 2008–31 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.

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE
—Particle Beam Science—

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

—Laser Matter Interaction Science—

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

Sakabe S, Emonstration of Ultra-fast Electron Diffraction Using Electrons Accelerated in Plasmas Produced by an Intense Short Pulse Laser, Yamada Science Foundation, 1 April 2010 –31 March 2012.

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

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

Hashida M, Improvement of Ablation Rate for Femtosecond Laser Processing, Amada Foundation for Metal Work Technology, 14 December 2007–31 March 2010.

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

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

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.

—Electron Microscopy and Crystal Chemistry—

Kurata H, Local State Analysis of Defects and Interface Regions by Sphencial Aberration Corrected STEM and EELS, Grant-in-Aid for Scientific Research (B), 1 April 2007–31 March 2010.

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

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

—Organic Main Group Chemistry—

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

—Advanced Solid State Chemistry—

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

—Organotransition Metal Chemistry—

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.

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.

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.

—Photonic Elements Science—

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

BIOINFORMATICS CENTER

—Bioknowledge Systems—

Kanehisa M, Backbone Database for Analysis of the Biological Systems and Environment, Grant-in-Aid for Scientific Research on Priority Areas, MEXT, 1 April 2005–31 March 2010.

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

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

—Biological Information Networks—

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

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

—Pathway Engineering—

Mamitsuka H, Integrative Mining from Semi-structured Data in Life Sciences, Institute for Bioinformatics and Research Development, Japan Science and Technology Agency, 1 October 2007–30 September 2010.

ENDOWED RESEARCH SECTION

—Water Chemistry Energy (AGC) —

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.

THESES

AMR, Mohammed Hassan
D Agr, Kyoto University
“Studies of Novel Enzymes Involved in Metabolism of 2-Chloroacrylic Acid”
Supervisor: Assoc Prof KURIHARA, Tatsuo
24 September 2010

BROWN, John
D Inf, Kyoto University
“Kernel Methods in Biochemical Informatics and Applications to DNA Repair Research”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2010

DELMO, Michael Picazo
D Sc, Kyoto University
“Large Magnetoresistance Effect in Silicon in Non-Ohmic Transport Regimes”
Supervisor: Assoc Prof KOBAYASHI, Kensuke
23 March 2010

HARUTA, Mitsutaka
D Sc, Kyoto University
“Development and Application of Site-resolved Analysis by HAADF-STEM Method”
Supervisor: Assoc Prof KURATA, Hiroki
23 March 2010

HIRANO, Daisuke
D Sc, Kyoto University
“Photoluminescence Dynamics of Highly Dense Excitons in Wide-band-gap Semiconductor Mixed Crystals”
Supervisor: Assoc Prof MATSUDA, Kazunari
23 March 2010

INAMURA, Koji
D Sc, Kyoto University
“Elucidation of the Properties of Stable Phenanthrenes Containing a Heavier Group 14 Element”
Supervisor: Prof TOKITOH, Norihiro
23 March 2010

KAWAI, Masanori
D Sc, Kyoto University
“Investigations of Resistance Switching Phenomena Observed for Epitaxially-grown Transition Metal Oxide Thin Films”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2010

MATSUMOTO, Teruyuki
D Sc, Kyoto University
“Studies on Novel Monoanionic Bidentate Ligands Bearing a Low-coordinated Phosphorus Atom”
Supervisor: Prof TOKITOH, Norihiro
23 March 2010

MORISAKI, Tatsuya
D Pharm Sc, Kyoto University
“DNA Binding Kinetics of Multi-Zinc Finger Proteins in Living Cells”
Supervisor: Prof FUTAKI, Shiroh
23 March 2010

NAKAGAWA, Yusuke
D Sc, Kyoto University
“Stable Isotope Marine Geochemistry of Molybdenum and Tungsten”
Supervisor: Prof SOHRIN, Yoshiki
23 March 2010

OKA, Kengo
D Sc, Kyoto University
“Investigations on Structural and Physical Properties of Pb or Bi-based Perovskite Oxides”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2010

TAKARABE, Masataka
D Pharm Sc, Kyoto University
“Network-based Analysis and Characterization of Drug Interactions”
Supervisor: Prof KANEHISA, Minoru
23 March 2010

TAMADA, Yoshinori
D Sc, Kyoto University
“Synthesis and Characterization of Magnetic Metallic Nanoparticles”
Supervisor: Prof ONO, Teruo
23 March 2010

TANABE, Yusuke
D Sc, Kyoto University
“New Aspects in the Chemistry of Silaaromatic Compounds and Coordination Chemistry Based on SiC_5 Ring Skeletons”
Supervisor: Prof TOKITOH, Norihiro
23 March 2010

TANAKA, Michihiro
D Pharm Sc, Kyoto University
“Analysis of the Relationship between Eukaryote Genomes and Lipid Molecular Species”
Supervisor: Prof KANEHISA, Minoru
23 March 2010

TANIGUCHI Y, Yukimi
D Sc, Kyoto University
“Biological Function of the *Phospholipase Dξ2* Gene of *Arabidopsis thaliana*”
Supervisor: Prof AOYAMA, Takashi
23 March 2010

TSURUSAKI, Akihiro
D Sc, Kyoto University
“Studies on the Construction of Extended π-Electron Conjugated Systems Bearing a Diphosphene Unit”
Supervisor: Prof TOKITOH, Norihiro
23 March 2010

URUNO, Yoshiharu
D Pharm Sc, Kyoto University
“Creation of Novel Substances Based on Architecture of D, L-Alternating Oligomers”
Supervisor: Prof KAWABATA, Takeo
23 March 2010

YAMAUCHI, Yoshiaki
D Sc, Kyoto University
“Experimental Study on the Quantum Coherence in Semiconductor Electron Interferometers”
Supervisor: Assoc Prof KOBAYASHI, Kensuke
23 March 2010

YAMAZOE, Sayumi
D Med Sc, Kyoto University
“A Dumbbell-Shaped Small Molecule that Promotes Cell Adhesion and Growth”
Supervisor: Prof UESUGI, Motonari
23 January 2010

ZHANG, Wanjiao
D Agr, Kyoto University
“Studies on Biosynthesis of Sulfur- and Selenium-Containing Molecules in Bacteria”
Supervisor: Assoc Prof KURIHARA, Tatsuo
23 March 2010

THE 110TH
ICR ANNUAL
SYMPOSIUM

SEMINARS
MEETINGS AND
SYMPOSIA

THE 110TH ICR ANNUAL SYMPOSIUM

(10 December 2010)

ORAL PRESENTATIONS

NAKAMURA, Yasuyuki (Polymer Controlled Synthesis)
“Living Radical Polymerization Using Organotelluriums: Photo-Polymerization and Control of Polymer Chain End Structure”

NAKAJIMA, Yumiko (Organotransition Metal Chemistry)
“Synthesis and Properties of 3d Metal Complexes Bearing a Bis(phosphaethenyl)pyridine Ligand”

ICHIKAWA, Noriya (Advanced Solid State Chemistry)
“Changes of Structure and Property in Thin Films of Transition Metal Oxides Due to Low-temperature Reduction/Oxidation”

TAKARABE, Masataka et al. (Bioknowledge Systems)
“Network-based Analysis and Characterization of Drug Interactions”

SEIKE, Hirofumi et al. (Organic Main Group Chemistry)
“Nickel-Catalyzed Alkenylative Cross-Coupling Reaction of Alkyl Sulfides”

IMANISHI, Miki (Biofunctional Design-Chemistry)
“Creation of Artificial Transcription Factors towards Control of Biological Activities”

TSUJII, Yoshinobu (Chemistry of Polymer Materials)
“Materials Design by Living Radical Polymerization: New Functions via Structural Control”

– ICR Award for Young Scientists –
MIZUHATA, Yoshiyuki (Organoelement Chemistry)
“1,2-Dialkynyldisilenes: Silicon Analogues of (*E*)-Enediyne”

– ICR Award for Graduate Students –
HASHIMOTO, Toru (Organic Main Group Chemistry)
“Iron-Catalyzed Suzuki-Miyaura Coupling of Alkyl Halides”

NAKAMURA, Shuji (Nanospintronics)
“Nonequilibrium Fluctuation Relations in a Quantum Coherent Conductor”

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

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

GE SUGAMATA, Koh; SASAMORI, Takahiro; TOKITOH, Norihiro
“Synthesis and Structures of Various Type of Organotellurium Halides”

GE SATO, Takahiro; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“Syntheses and Properties of Trimethylsilyl- and Phenyl-substituted 1,2-Dialkynyldisilenes”

— Structural Organic Chemistry —

LW “Recent Research in Structural Organic Chemistry Laboratory”

GE NOBORI, Masahiro; MURATA, Michihisa; MURATA, Yasujiro
“Investigation on Magnetic Properties of Fullerenes with Encapsulated Dihydrogen”

GE KATSUYA, Satoshi; MURATA, Michihisa; MURATA, Yasujiro
“Studies on Synthesis of Azafullerene Derivatives Directly Connected to Organic Dyes”

— Synthetic Organic Chemistry —

GE HAYASHI, Kazuhiro; MATUBAYASI, Nobuyuki; YOSHIMURA, Tomoyuki; SASAMORI, Takahiro; TOKITOH, Norihiro; KAWABATA, Takeo
“Creation of Chiral Binaphthyl Surrogates with an Intramolecular Hydrogen Bond, and Its Application to Novel Organometallic Catalysis”

GE YOSHIDA, Keisuke; FURUTA, Takumi; KAWABATA, Takeo
“Regioselective Monoacylation of 2-amino-1,5-pentanediols by PPY Catalysts with Functional Side Chains”

— Chemistry of Polymer Materials —

LT HUANG, Yun; SASANO, Tatsuya; OHNO, Kohji; TSUJII, Yoshinobu
“Well-organized Assemblies of Hybrid Particles Grafted with Concentrated Polymer Brush”

GE NAKANISHI, Yohei; KAWANO, Yuko; OHNO, Koji; TSUJII, Yoshinobu; SAGAWA, Takashi; YOSHIKAWA, Susumu; SATO, Takaya
“Development of Dye-sensitized Solar Cells Based on Novel Solid-state Electrolyte”

— Polymer Controlled Synthesis —

LW “Research Activity of Polymer Controlled Synthesis Laboratory”

GE MISHIMA, Eri; YAMAGO, Shigeru
“Synthesis of Novel Random and Block Copolymers by Organotellurium-Mediated Controlled / Living Radical Polymerization of (Meth)acrylates and Vinyl Ethers”

GE KONISHI, Shota; KAYAHARA, Eiichi; YAMAGO, Shigeru; NOMURA, Akihiro; GOTO, Atsushi; TSUJII, Yoshinobu
“Synthesis of Concentrated Polymer Brush via Surface-Initiated TERP”

GE IWAMOTO, Takahiro; WATANABE, Yoshiki; YAMAGO, Shigeru
“Synthesis of Cycloparaphenylenes and Their Derivatives from Square-Shaped Tetranuclear Platinum Complexes”

GE KITADA, Yukie; NAKAMURA, Yasuyuki; KOBAYASHI, Yu; RAY, Biswajit; YAMAGO, Shigeru
“Quantitative Analysis of the Effect of AIBN in Organoheteroatom-mediated Living Radical Polymerization”

— Inorganic Photonics Materials —

LT NISHIOKA, Satoshi; TOKUDA, Yomei; TAKAHASHI, Masahide; UEDA, Yoshikatu; YOKO, Toshinobu
“Preparation of Organic-inorganic Hybrid Titanophosphite Membranes with Proton Conductivity”

LT YAMAMOTO, Kazuyuki; TOKUDA, Yomei; CRISTIANA, Figus; TONGJIT, Kichob; PLINIO, Innocenzi; TAKAHASHI, Masahide; YOKO, Toshinobu
“Preparation of Organic-inorganic Hybrid Hollow Fiber by Self-organization”

LT YAMAMOTO, Taiga; TOKUDA, Yomei; MASAI, Hirokazu; TAKAHASHI, Masahide; YOKO, Toshinobu
“The Synthesis of Organic-inorganic Hybrid Low-melting Glasses Using Photochemical Reaction”

— Nanospintronics —

GE KOYAMA, Tomohiro
“Current-induced Magnetic Domain Wall Motion in Perpendiculary Magnetized Nano-wire”

GE NAKANO, Kunihiro
“Real-time Detection of the Vortex Core Resonance Motion”

— Biofunctional Design-Chemistry —

LW “Research Topics in Biofunctional Design Chemistry Laboratory”

GE TANAKA, Gen; NAKASE, Ikuhiko; FUKUDA, Yasunori; FUTAKI, Shiroh
“Identification of Potential Receptor that Stimulates the Cellular Uptake of the Arginine-rich Peptides”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities of Laboratory of Chemistry of Molecular Biocatalysts”

GE IKEUCHI, Hideyuki; OTOKAWA, Takuya; WATANABE, Bunta; HIRATAKE, Jun
“Synthesis of Asparagine Synthetase Inhibitors -Synthesis of New Therapeutic Agent for ALL-”

— Molecular Biology —

LW “Research of the Molecular Biology Laboratory”

— Chemical Biology —

LW “Chemical Biology”

— Molecular Materials Chemistry —

LT FUKUCHI, Masashi; FUKUSHIMA, Tatsuya; GOTO, Atsushi; KAJI, Hironori
“Analysis of Molecular Orientation in Polyfluorene Films by Solid-state NMR”

GE TOKUDOME, Yasuaki; NAKANISHI, Kazuki; KOSAKA, Sho; KARIYA, Ayuta; HANADA, Teiichi; KAJI, Hironori
“Synthesis of High-silica and Low-silica Zeolite Monoliths with Trimodal Pores”

— Hydrospheric Environment Analytical Chemistry —

LW “Recent Research Topics from Hydrospheric Environment-Analytical Chemistry”

GE WATANABE, Kazuya; UMETANI, Shigeo; SOHRIN, Yoshiki
“Cu(II) or Pd(II) Imprinted Adsorbents for the Separation of Metal Ions”

— Solution and Interface Chemistry —

LT SHINTANI, Megumi
“NMR-NOE and MD Simulation Study on Intermolecular Interaction and Dynamics of Lipid Membranes with Different Curvature”

GE KIMURA, Hiroshi
“Mechanisms and Kinetics for Hydrothermal Decomposition of Glucose”

— Molecular Microbial Science —

LW “Introduction of Molecular Microbial Science Lab.”

— Polymer Materials Science —

LW “Recent Research Topics in Polymer Material Science Laboratory”

LT MATSUI, Kazuya
“Phase Separation and Dewetting Process of Polymer Blend Thin Film as Studied by Neutron Reflectivity”

GE MATSUMOTO, Norihiro
“Crystallization of Poly(Butylene-2,6-Naphthalate) through the Mesomorphic Phase”

GE FUJIWARA, Tetsuaki
“Precursor of Shish-kebab in Isotactic Polystyrene Induced by Shear Flow”

— Molecular Rheology —

LW “Laboratory of Molecular Rheology”

— Molecular Aggregation Analysis —

LT YOSHIDA, Hiroyuki; SATO, Naoki
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