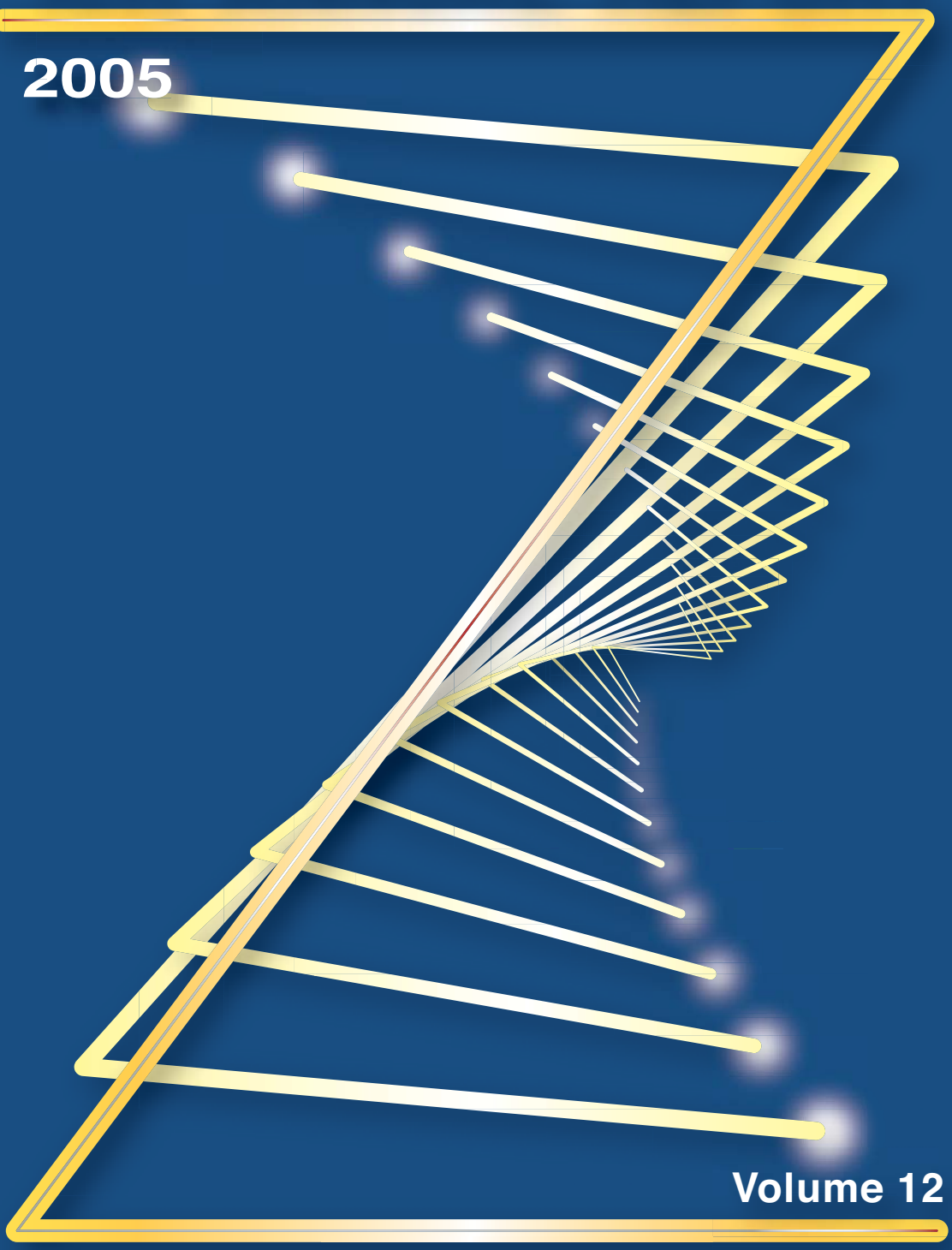
ISSN 1342-0321
IAREFM

ICR ANNUAL REPORT

2005



Volume 12

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2005 (Volume 12) - ISSN 1342-0321 -
This Annual Report covers from 1 January to 31 December 2005

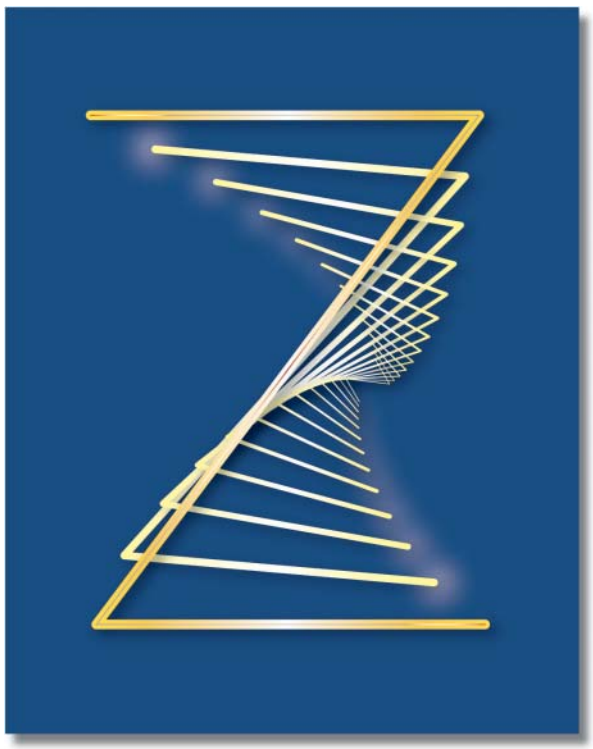
Published and Distributed by:
Institute for Chemical Research (*ICR*), Kyoto University

Note: *ICR* Annual Report available from the *ICR* Office,
Institute for Chemical Research, Kyoto University,
Gokasho, Uji, Kyoto 611-0011, Japan
Tel: +81-(0)774-38-3344
Fax: +81-(0)774-38-3014
E-mail koho@scl.kyoto-u.ac.jp
URL http://www.kuicr.kyoto-u.ac.jp/index.html

Uji Library, Kyoto University
Tel: +81-(0)774-38-3011
Fax: +81-(0)774-38-4370
E-mail ujibunkan@kulib.kyoto-u.ac.jp
URL http://lib.kuicr.kyoto-u.ac.jp/homepage/english/homepageeng.html

Printed by:
Nakanishi Printing Co., Ltd.
Ogawa Higashi-iru, Shimodachiuri, Kamigyo-ku, Kyoto 602-8048, Japan
TEL:+81-(0)75-441-3155 FAX:+81-(0)75-417-2050

ICR ANNUAL REPORT 2005



Institute for Chemical Research
Kyoto University
Volume 12

Preface

Institute for Chemical Research at Kyoto University has celebrated its 79th anniversary in October 2005. Initially, the size of the Institute was not substantial and it contained only a limited number of laboratories, but growth soon accelerated. In 1962, the Institute accepted its first graduate students, and, in 1964, a new research-division structure was introduced, establishing the foundation for the present organization. Through radical organizational changes in 1992, and restructuring in 2004, we have finally reached the current large-scale organization of three centers and five research divisions. Under this system, we have three leading-edge centers: the Bioinformatics Center, the International Research Center for Element Science, and the Advanced Research Center for Beam Science. Currently, 104 faculty members and 240 graduate students are engaged in research activities in 31 laboratories supervised by full-time professors and five laboratories supervised by visiting professors.

Our founding vision is to "Excel in the investigation of basic principles of chemistry and chemical applications." This legacy continues to the present day and describes the essence of our research activities. With this vision in mind, we have entrusted our scientists to choose and pursue research topics at the forefront of advanced chemistry with bottom-up paradigms; this has resulted in substantial contributions to the development of scientific technology. Such accomplishments are proof of our vision of freedom and a bottom-up approach in chemical research.

The research within the Institute encompasses the fields of chemistry, physics, biology, and informatics. The chemical studies core covers fields including physical chemistry, inorganic chemistry, organic chemistry, materials chemistry, and biochemistry. The graduate school to which our laboratories belong spans diverse fields of science, engineering, agriculture, pharmaceutical sciences, medicine, informatics, and human/environmental studies. The labs at the graduate school are spearheading leading-edge research, and yielding outstanding results in their own research areas. The Institute is currently performing research activities either as the head or as a core member of three 21st Century Center of Excellence (COE) projects in the fields of chemistry, physics, and the interdisciplinary area of bioinformatics and pharmaceutical sciences. In addition, we are expanding our global research by pro-actively recruiting researchers and students from abroad and promoting joint research programs with overseas entities. Moreover, we are encouraging community education to communicate the significance and appeal of cutting-edge research through our "Chemical Research for High School Students" and "Open Campus" programs.

Under the recently enacted statute of incorporation of universities, each university realizes the importance of balancing competition and collaboration, and searches for strong liaisons with other universities that create uniqueness within the framework of a competitive environment. We are genuinely pleased to announce the acceptance of a proposal for a Center of Excellence project concerning material synthesis made by the International Research Center for Elements Science at Kyoto University in collaboration with the Research Center for Materials Science at Nagoya University and the Institute for Materials Chemistry and Engineering at Kyushu University; this COE project has initiated active research activities in 2005. These three centers for chemical research, which were established as a direct outcome of the COE program, are willing to share research resources and collaborate, in order to form and maintain an open and interdisciplinary chemical research center. Furthermore, we believe that our plan will become a model for cooperation in science, a desirable outcome of the recent university incorporation.

Whether or not the human race can generate sustainable growth is a key issue of the 21st century. Therefore, in the Institute for Chemical Research, in order to contribute to the future of our society, we encourage our scientists to be actively involved in research projects with bottom-up approach in mind, and to value the emergence of unique interdisciplinary research projects. Upon embracing the second year of incorporation of universities, and to further reinforce the leadership of the Institute, we are pleased to announce the appointments of Prof. Naoki Sato and Prof. Norihiro Tokitoh as Vice Directors. Under this new administration, we shall strive to further encourage the research activities and install effective management at the Institute.

Finally, we appreciate your continued encouragement and support.

January 2006

ESAKI, Nobuyoshi
Director

ICR News 2005

The Newly Constructed "Uji Research Building," Home for the Bioinformatics Center

Director of Bioinformatics Center:
Prof KANEHISA, Minoru

Uji Research Building

GenomeNet Server on the first floor

The Bioinformatics Center moved into the new Uji Research Building in November, 2004. Being involved in the 21st Century COE Program, "Knowledge Information Infrastructure for Genome Science" with the School of Pharmaceutical Sciences, a lecture room installed with a distance-learning system and a computer room for laboratory training are set up on the second floor for this and other projects. The Bioinformatics Center provides the KEGG database resource as well as GenomeNet, which is the most prominent bio-data service in Japan. The KEGG development room, the GenomeNet operating room, and the supercomputer laboratory maintenance room are located on the second floor. The supercomputer system for the Institute for Chemical Research, the central computer system, and the servers for the Bioinformatics Center are on the first floor in the main computer room. Computing and database services for all of Kyoto University as well as the GenomeNet services are provided by these machines.

Lecture room with a distance-learning system

Speech addressed by President Oike of Kyoto University, at the completion ceremony of the Uji Research Building.

http://www.bic.kyoto-u.ac.jp/

“Joint Project of Chemical Synthesis Core Research Institutions”

Research and Education Funding for Inter-University Research Project, MEXT, Japan (2005–2010)

■ Director of IRCELS: Prof OZAWA, Fumiyuki

Organization

Elements Chemistry Research Unit:
Institute for Chemical Research, Kyoto University

Functional Molecular Chemistry Research Unit:
Research Center for Materials Science, Nagoya University

Assembled Molecular Chemistry Research Unit:
Institute for Materials Chemistry and Engineering, Kyushu University

Opening Ceremony of the Joint Project (30 June 2005, at Nagoya University)

■ http://www.kuicr.kyoto-u.ac.jp/IRCELS/index_e.html

Future advances in chemical synthesis will be fueled by a strong cooperative and collaborative research program. 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 three 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.

A Novel Style of “Periodic Table of the Elements” Has Been Made in Cooperation with the MEXT

■ Prof YOKO, Toshinobu

“Periodic Table of the Elements” that has long been thought to be boring and uninteresting has been renewed by Prof. Tamao, a former director of ICR, and his colleagues, who worry about the recent tendency of Japanese young people’s losing interest in science, on the basis of the following unique concepts;

- Decoration of the wall of a living room at home with a beautiful sheet of “Periodic Table of the Elements”.
- Conversation with a family about scientific topics with a family looking at such a quite obvious beautiful lofty sheet.
- Memorization of the catch phrase that “nature, a life, and our body all are written by the symbol of an element”.
- Recognition of the benefit of science and technology in everyday life from childhood.

It is eagerly desired that the children who get interested in science and aim at being a chemist increase rapidly in number due to the “Prof. Tamao’s Periodic Table of the Elements”.

■ http://stw.mext.go.jp/

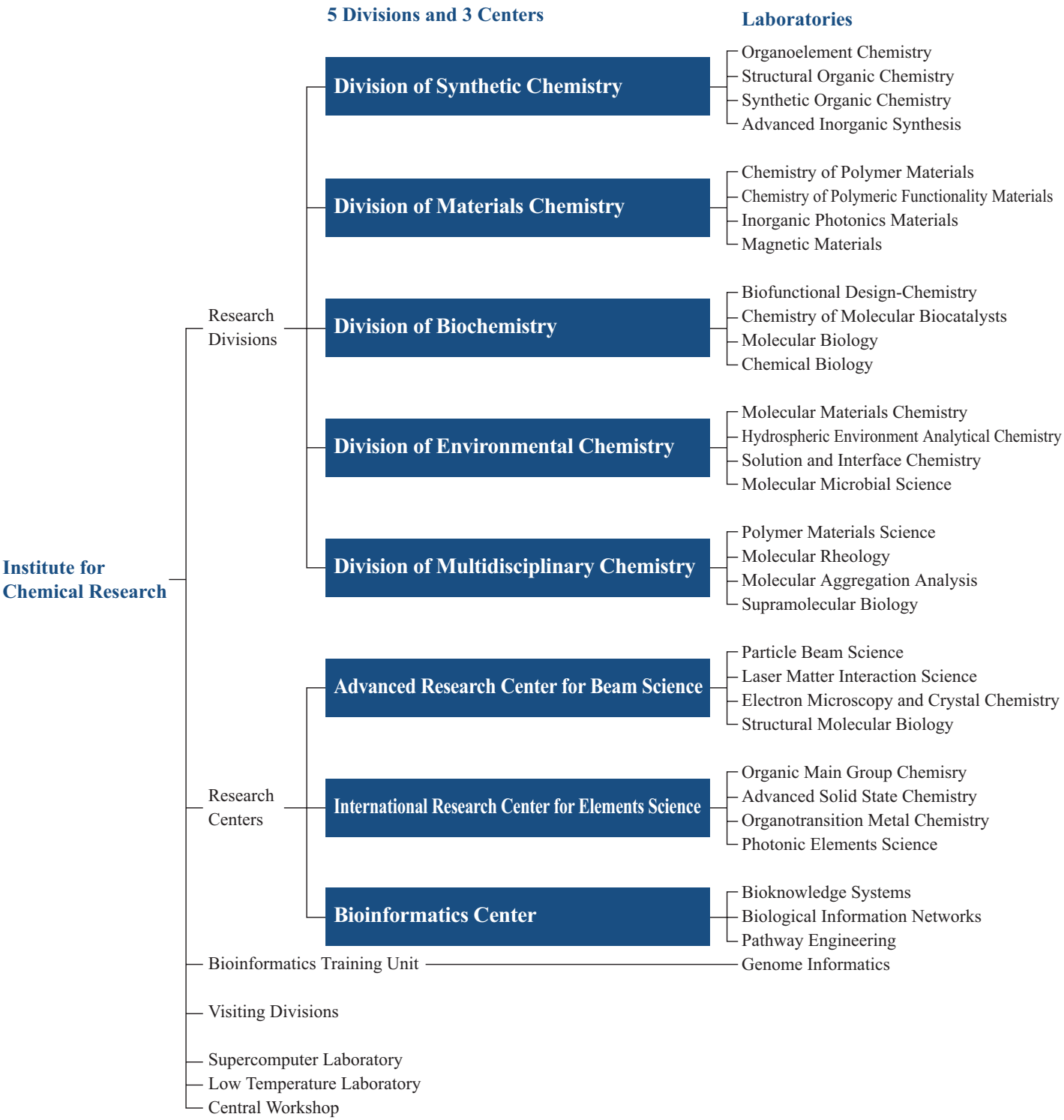
CONTENTS

Abbreviations used in the columns

Prof Em	Professor Emeritus
Prof	Professor
Vis Prof	Visiting Professor
Assoc Prof	Associate Professor
Vis Assoc Prof	Visiting Associate Professor
Lect	Lecturer
Assist Prof	Assistant Professor
Vis Assist Prof	Visiting Assistant Professor
Res Associate	Research Associate
Techn	Technician
Guest Scholar	Guest Scholar
Guest Res Assoc	Guest Research Associate
PD	Post-Doctoral Research Fellow
Res	Researcher
A Res	Assistant Researcher

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
(REF)	Resarch and Education Funding
(NEDO)	New Energy and Industrial Technology Development Organization
(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
Chemistry of Polymeric Functionality Materials
Inorganic Photonics Materials
Magnetic Materials
Division of Biochemistry
Biofunctional Design-Chemistry
Chemistry of Molecular Biocatalysts
Molecular Biology
Chemical Biology
Division of Environmental Chemistry
Molecular Materials Chemistry
Hydrospheric Environment Analytical Chemistry
Solution and Interface Chemistry
Molecular Microbial Science
Division of Multidisciplinary Chemistry
Polymer Materials Science
Molecular Rheology
Molecular Aggregation Analysis
Supramolecular Biology
Research Centers
Advanced Research Center for Beam Science
Particle Beam Science
Laser Matter Interaction Science
Electron Microscopy and Crystal Chemistry
Structural Molecular Biology
International Research Center for Elements Science
Organic Main Group Chemisry
Advanced Solid State Chemistry
Organotransition Metal Chemistry
Photonic Elements Science
Bioinformatics Center
Bioknowledge Systems
Biological Information Networks
Pathway Engineering
Bioinformatics Training Unit
Genome Informatics
Visiting Divisions
Supercomputer Laboratory
Low Temperature Laboratory
Central Workshop

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry
- Organoelement Chemistry -

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

Prof
TOKITOH, Norihiro
(D Sc)

Assoc Prof
NAKAMURA, Kaoru
(D Sc)

Assist Prof
TAKEDA, Nobuhiro
(D Sc)

Assist Prof
SASAMORI, Takahiro
(D Sc)

Techn
HIRANO, Toshiko

A Res
NAGAHORA, Noriyoshi
(D Eng)

Res
TAJIMA, Tomoyuki
(D Sc)

Students

SHIMIZU, Daisuke (D3)
SUGIYAMA, Yusuke (D3)
MIZUHATA, Yoshiyuki (D3)
KOBAYASHI, Megumi (D2)
HAMAKI, Hirofumi (D2)
ISOBE, Toru (D1)
MATSUMOTO, Takeshi (D1)
OZAKI, Shuhei (M2)
KAWAI, Masahiro (M2)
TANABE, Taro (M2)
INAMURA, Koji (M1)
TSURUSAKI, Akihiro (M1)
MATSUMOTO, Teruyuki (M1)

Visitor

Prof DRIESS, Matthias Technical University Berlin, Germany, 30 November - 1 December 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Some Unique Reactions of Kinetically Stabilized Silaaromatic Compounds with Haloalkanes and Polyaromatic Hydrocarbons, Tokitoh N, Shinohara A, Takeda N, Sasamori T, 14th International Symposium on Organosilicon Chemistry (ISOS XIV), Würzburg, 31 July - 5 August 2005 (invited).

New Aspects in the Chemistry of Kinetically Stabilized Dipnictenes, Tokitoh N, Mieda E, Nagahora N, Sasamori T, Takeda N, Takagi N, Nagase S, 2005 International Chemical Congress of Pacific Basin Societies (Pacifichem 2005), Honolulu, 15 - 20 December 2005 (invited).

Grants

Tokitoh N, Takeda N, Sasamori T, 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 2009.

Tokitoh N, Synthesis of Dynamic Complexes Containing Heteroatoms by Taking Advantage of Kinetic Stabilization, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2002 - 31 March 2006.

Sasamori T, Synthesis of Novel π Electron Conjugated Systems Containing Heavier Group 14 and 15 Elements and the Elucidation of Their Properties, Grant-in-Aid for Young Scientists (B), 1 April 2004 - 31 March 2006.

Sasamori T, Synthesis of Novel Molecular Wire with π Electron Systems Containing Silicon and Phosphorus, Kinki Invention Center, 1 April 2005 - 31 March 2006.

Tajima T, Synthesis of Novel Chemical Species Containing a Heavier Group 14 Element by Taking Advantage of Dilithiometallanes Bearing a Bulky Substituent and Their Properties, Grant-in-Aid for JSPS Fellows, 1 April

Synthesis of the First Stable Stannaaromatic Compounds: 2-Stannanaphthalene

The chemistry of aromatic compounds containing a heavier group 14 element is important to understand the concept of "aromaticity", which has been one of the fascinating topics in organic chemistry. We have succeeded in the synthesis of kinetically stabilized sila- and germaaromatic compounds by taking advantage of an efficient steric protection group, 2,4,6-tris[bis(trimethylsilyl)methyl] phenyl (Tbt), and revealed their considerable aromaticity based on their molecular structures, spectroscopic properties, and reactivities. Recently, we have succeeded in the synthesis of the first stable neutral stannaaromatic compound, 2-stannanaphthalene **1**, 2-Stannanaphthalene **1** was synthesized by the dehydrobromination of the corresponding bromostannane **2** with LDA in hexane at –40°C. The NMR chemical shifts indicate the ring current effect on the 2-stannanaphthalene ring of **1**. The X-ray crystallographic analysis of **1** revealed the planar geometry of the 2-stannanaphthalene ring. All experimental results supported the aromatic character of **1**. In addition, 2-stannanaphthalene **1** was found to behave as an η^6-arene ligand in the ligand exchange reaction with $[Cr(CH_3CN)_3(CO)_3]$ giving the first stable η^6-2-stannanaphthalene chromium complex **3**.

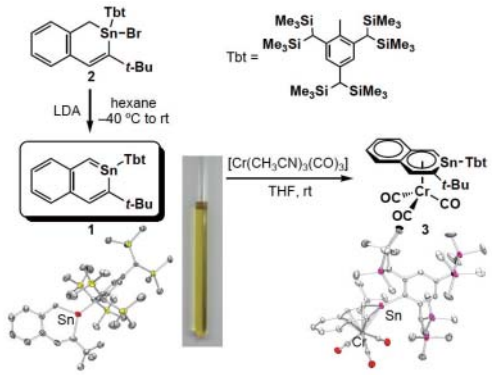


Figure 1. Syntheses of the first stable 2-stannanaphthalene **1** and its η^6-$Cr(CO)_3$ complex **3**.

Synthesis and Applications of New Polythioether Ligands Tethered with Bulky Substituents

The chemistry of cyclic polythioether ligands has been extensively studied, and it has been revealed that they can stabilize the metals with unusual valency, such as trivalent palladium. Acyclic polythioether ligands are also expected to show similar properties, however, the chemistry of acyclic polythioether ligands has been less explored.

New polythioether ligands **4** and **5** tethered with two Tbt groups were synthesized. Reactions of **4** with Na_2PdCl_4 gave a distorted octahedral palladium complex **6**. The X-ray structural analysis of **6** showed weak but distinct interactions between the terminal sulfur atoms and the central palladium atom (S•••Pd distances: 3.1755(8) Å).

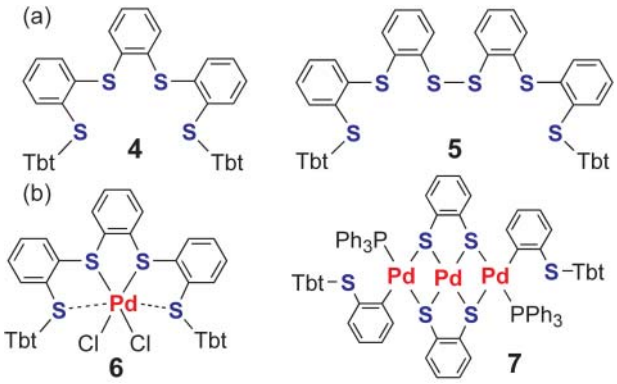


Figure 2. (a) Novel cyclic plythioether ligands **4** and **5**. (b) Structure of the $PdCl_2$ complex **6** and Pd trinuclear complex **7**.

Ligand **5** reacted with 3 molar amounts of $[Pd(PPh_3)_4]$ to give the trinuclear complex **7** in 58% yield. The formation of **7** can be explained in terms of the initial insertion of the Pd(0) atom to the S–S bond of **5** and the successive insertion of the two Pd(0) atoms to the C–S bonds.

2004 - 31 December 2005.

Mizuhata Y, Synthesis, Structure, and Properties of Kinetically Stabilized Tin-carbon Double-bond Compounds, Grant-in-Aid for JSPS Fellows, 1 April 2005 - 31 March 2007.

Awards

Sasamori T, Inoue Research Award for Young Scientists, Studies on the Synthesis of Low-coordinated Species of Heavier Group 15 Elements Utilizing Kinetic Stabilization, 4 February 2005.

Shinohara A, Takeda N, Sasamori T, Tokitoh N, BCSJ Award (The Best Article of the Month), Synthesis of Kinetically Stabilized 1-Silanaphthalenes and Their Properties, 15 June 2005.

Mizuhata Y, The Best Poster Award, Synthesis of a Stable 2-Stannanaphthalene and Its Structure and Properties, 10th Symposium of the Society of Silicon Chemistry, Japan, 28 October 2005.

Takeda N, The ICR Award for Yound Scientists, "Synthesis of Novel Organosilicon Species by Taking Advantage of a Silylene Bearing Bulky Substituents and the Elucidation of Their Properties", 2 December 2005.

Division of Synthetic Chemistry
- Structural Organic Chemistry -

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

Prof
KOMATSU, Koichi
(D Eng)

Assoc Prof
KITAGAWA, Toshikazu
(D Eng)

Assist Prof
MURATA, Yasujiro
(D Eng)

PD
MORI, Sadayuki
(D Eng)

PD
ISHIDA, Shintaro
(D Sc)

PD
NOGITA, Rika
(D Sc)

PD
MINEGISHI, Shinya
(Ph D)

PD
CHUANG, Shih-Ching
(Ph D)

Students

MIYATA, Yasuo (D3)
MURATA, Michihisa (D3)
YAMAZAKI, Daisuke (D2)
MAEDA, Shuhei (M2)
MATSUBARA, Hiroaki (M2)
TERAYAMA, Miki (M2)
TANABE, Fumiyuki (M1)
YOSHIDA, Ryohei (M1)
ISHIBASHI, Michinori (UG)
OCHI, Yuta (UG)

Visitor

Prof GLEITER, Rolf University of Heidelberg, Germany, 7 October - 6 November 2005

Scope of Research

Fundamental studies are being conducted for creation of new functional materials with novel structures and properties. The major subjects are: synthetic and structural studies on novel cyclic π-conjugated systems, particularly the positively charged species stabilized by σ-π interaction; synthesis of new redox-active and supramolecular π-systems; organo-chemical transformation of fullerenes C_{60} and C_{70}, specifically organic synthesis of endohedral fullerenes by the technique of molecular surgery; generation of alkylated C_{60} and C_{70} cations and their application for the synthesis of functional materials.

Research Activities (Year 2005)

Presentations

Organic Synthesis of Endohedral Fullerene Encapsulating Molecular Hydrogen, $H_2@C_{60}$, Komatsu K, The 19th International Winterschool on Electronic Properties of Novel Materials Euroconference (IWEPNM), 12 - 19 March 2005, Kirchberg, Austria.

Fullerene-Based New Materials Incorporating Molecular Hydrogen, Komatsu K, The Royal Society of Chemistry 7th International Conference on Materials Chemistry, 5 - 8 July 2005, Edinburgh, UK.

Novel Aromatics Blended with a σ-Flavor. (The Nozoe Lecture), Komatsu K, 11th International Symposium on Novel Aromatic Compounds, 14 August 2005, St. John's, Canada.

Generation and Properties of a Cyclopentadienyl Cation Annelated with Homoadamantene Frameworks, Kitagawa T, Ogawa K, Komatsu K, 11th International Symposium on Novel Aromatic Compounds, 17 August 2005, St. John's, Canada.

Organic Synthesis of an Endohedral Fullerene Encapsulating Molecular Hydrogen, $H_2@C_{60}$, Murata Y, Murata M, Komatsu K, The 4th International Symposium of the Kyoto COE Project "Elements Science", 6 January 2005, Kyoto.

Molecular Surgery Approach toward Organic Synthesis of Endohedral Fullerenes, Murata Y, International Symposium Next Generations and Perspectives of Organic Chemistry, 22 March 2005, Kyoto.

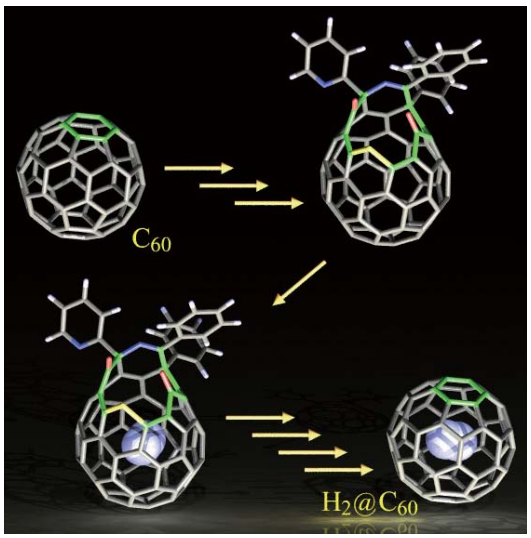
Properties of Open-Cage C_{70} Derivative Encapsulating Molecular Hydrogen, Murata Y, Maeda S, Murata M, Komatsu K, 207th Meeting of The Electrochemical Society, 18 May 2005, Quebec City, Canada.

Grants

Komatsu K, Grant-in-Aid for Scientific Research (B), Development of Organic Synthetic Method for Endohedral

Synthesis of H_2@C_{60} by "Molecular Surgery"

The "molecular surgery" of fullerenes involves making an orifice on a fullerene cage, insertion of a guest through the orifice, and closure of the orifice using the technique of organic synthesis. A C_{60} derivative having a 13-membered-ring orifice was synthesized by three-step organic reactions in 40% yield. The 100% encapsulation of a hydrogen molecule inside the fullerene cage was attained under high-pressure. Closure of the orifice with retention of the encapsulation was achieved by four-step organic reactions in 22% yield. Thus, H_2@C_{60} was isolated as thermally stable powder for the first time[1].

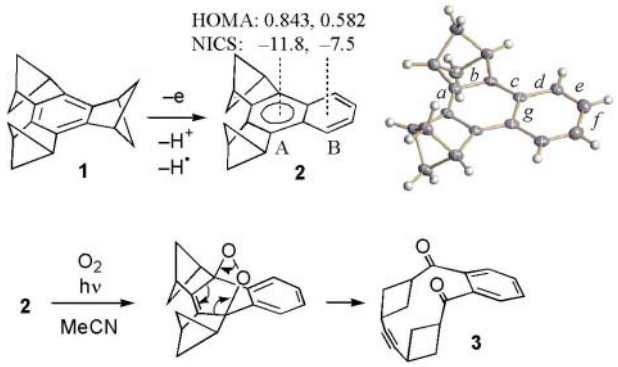


Stable Alkylated C_{70} Cation

The first monoalkylated C_{70} cation, $CHCl_2$-C_{70}^+ was generated by ionization of the fullerenol $CHCl_2$-C_{70}-OH in CF_3SO_3H at room temperature and was observed by NMR as a long-lived carbocation. The obtained new cation consisted of a single regioisomer, the structure of which was determined by ^{1}H and ^{13}C NMR analyses and DFT calculations. The stability of $CHCl_2$-C_{70}^+ was found to be comparable to that of the C_{60} analogue, $CHCl_2$-C_{60}^+, and tert-butyl cation, based on the thermodynamic parameters obtained by kinetic measurements of the solvolysis of the chloride $CHCl_2$-C_{70}-Cl[2].

A Naphthalene with Unusual Bond Alternation

A novel naphthalene **2** annelated with two bicyclo[2.1.1]-hexene (BCH) units at ring A was obtained by one-electron oxidation of bond-fixed benzene **1** having three BCH units. In contrast to benzene **1**, the X-ray crystallography demonstrated bond equalization in ring A and strong bond fixation in ring B (*a*, 1.384 Å; *b*, 1.394 Å; *c*, 1.395 Å; *d*, 1.430 Å; *e*, 1.356 Å; *f*, 1.414 Å; *g*, 1.447 Å). This is reflected in much greater aromaticity in ring A as shown by theoretical calculations of HOMA and NICS values. In spite of the increased aromaticity, ring A exhibited higher reactivity toward singlet oxygen due to the inherent strain, and quantitatively afforded macrocyclic diketone **3** containing a triple bond[3].



[1] Komatsu, K.; Murata, M.; Murata, Y. *Science* **2005**, *307*, 238-240.
[2] Kitagawa, T.; Lee, Y.; Masaoka, N.; Komatsu, K. *Angew. Chem. Int. Ed.* **2005**, *44*, 1398-1401.
[3] Uto, T.; Nishinaga, T.; Matsuura, A.; Inoue, R.; Komatsu, K. *J. Am. Chem. Soc.* **2005**, *127*, 10162-10163.

Fullerenes, April 2004 - March 2006.

Kitagawa T, Grant-in-Aid for Scientific Research (C) (2), April 2004 - March 2006.

Kitagawa T, CREST, Japan Science and Technology Agency, November 2002 - October 2007.

Murata Y, Grant-in-Aid for Young Scientists (A), April 2004 - March 2007.

Murata Y, Komatsu K, Academic-Industrial Cooperative Research Fund, April 2005 - March 2006.

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

Awards

Murata M, The Best Oral Presentation Award, The First Synthesis of Fullerene C_{60} Encapsulating Molecular Hydrogen, The 85th Annual Meeting of the Chemical Society of Japan, April 2005.

Murata M, The ICR Award for Students, Organic Synthesis of Fullerene C_{60} Encapsulating Molecular Hydrogen, ICR, 2 December 2005.

Division of Synthetic Chemistry
- Synthetic Organic Chemistry -

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

Prof
KAWABATA, Takeo
(D Phram Sc)

Assoc Prof
TSUBAKI, Kazunori
(D Pharm Sc)

Res Associate
YOSHIMURA, Tomoyuki
(D Pharm Sc)

Techn
TERADA, Tomoko

PD
JIANG, Changsheng
(Ph D)

PD
REDDY, Valluru Krishna
(Ph D)

PD
HAI, Dinh Thi Thanh
(Ph D)

Students

MONGUCHI, Daiki (D2)
MORIYAMA, Katsuhiko (D2)
TANIMA, Daisuke (D2)
MURAMATSU, Wataru (D1)
TAKAISHI, Kazuto (D1)
TERAOKA, Fumiteru (D1)
NAKATANI, Yuki (M2)
WATANABE, Toshihide (M2)
MATSUDA, Seiji (M1)
SAKAKIBARA, Masahide (M1)
SHIBATA, Takeshi (M1)
URUNO, Yoshiharu (M1)
HAYASHI, Kazuhiro (UG)
OKA, Takahiro (RF)

Visitors

Prof PARMER, Virinder S. University of Dehli, India, 25 March 2005
Prof ZIPSE, Hendrik Ludwig-Maximilians-Univeisität in München, Germany, 16 September 2005

Scope of Research

The research interests of the laboratory include the development of advanced molecular transformation, total synthesis of biologically active products, and molecular recognition. Programs are active in the areas of asymmetric alkylation of carbonyl compounds based on “memory of chirality”, nucleophilic catalysis for fine organic syntheis, synthesis of unusual amino acids and nitrogen heterocycles, visualization of molecular information by functionalized phenolphthaleins, use of homooxacalixarene for molecular recognition, and the structural and functional investigation of homo-and heterochiral oligomers.

Research Activities (Year 2005)

Presentations

Design and Development of the Asymmetric Reactions Based on Memory of Chirality, Kawabata T, 125th Annual Meeting of the Pharmaceutical Society of Japan, 29 March.

Enantioselective Acceleration in Asymmetric Acylation of Alcohols Promoted by Chiral Nucleophilic Catalysts, Kawabata T, Molecular Chirality 2005, 7 June.

Temperature-Dependent Coloration of Phenolphthalein Derivatives with Alkali Metals, Tanima D, 35th Symposium on Structural Organic Chemistry, 9 September.

Memory of Chirality at Room Temperature, Monguchi D, 31st Symposium on Progress in Organic Reactions and Syntheses, 7 November.

Stereochemical Reversal in Asymmetric Cyclization via Memory of Chirality, Kawabata T, Pacifichem 2005, 15 December.

Grants

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

Tsubaki K, Synthesis and Properties of Optically Active Oligonaphthalene Derivatives, Grant-in-Aid for Exploratory Research, 1 April 2005 - 31 March 2007.

Kawabata T, Synthesis of Highly Functionalized Heterocycles by Asymmetric Cyclization via Memory of Chirality, Grant-in-Aid for Scientific Research, 30 September 2005 - 29 September 2007.

Kawabata T, Development of C_2-Symmetric Chiral Nucleophilic Catalysts and their Use in Asymmetric C-C Bond Formation, Grant-in-Aid for Scientific Research, 25 June 2004 - 24 June 2006.

Kawabata T, Design of a New Generation of Nucleophilic Catalysts and Selective Reactions, Grant-in-Aid for

An X-Ray Structure of an Axially Chiral Enolate

An X-ray crystal structural analysis of an axially chiral enolate has been performed for the first time. A single crystal of a lithium enolate formed by treatment of valine derivative **1** with lithium hexamethyldisilazide (LHMDS) in a mixture of pentane and *t*-butyl methyl ether at 0°C. The tetrameric Li enolate has a cubic core consisting of four Li and four O atoms surrounded by four enolate subunits (Figure 1, a). Configuration of the tetrameric enolate is (a*S*,a*S*,a*R*,a*R*), which is the result of racemization of chiral C-N axes due to high temperature (0°C) employed for the enolate formation. The nitrogen atom of the enolate is almost completely planar (Figure 1, b). A plane consisting of the planar nitrogen and the substituents forms an angle of 105.2° with that of an enolate plane. This clearly indicates axial chirality of the enolate structure in a solid state. We had already proposed, based on kinetic data, an axially chiral nonracemic enolate intermediate as a crucial intermediate for the asymmetric induction via memory of chirality. This crystal structure is the first concrete evidence for an axially chiral enolate.

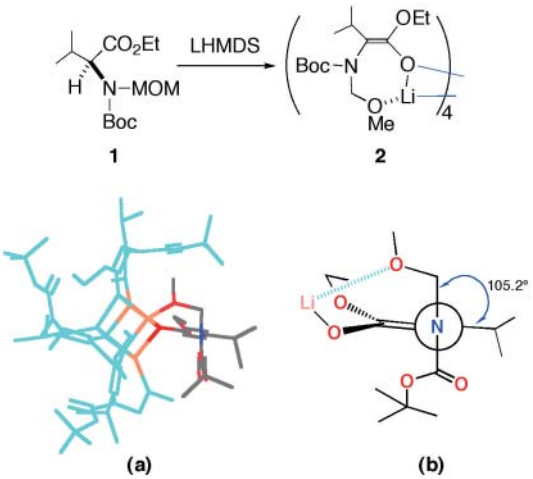
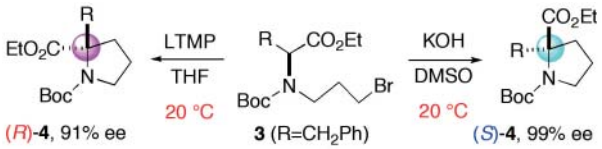


Figure 1. (a) X-ray structure of **2**. An enolate unit of the tetrameric enolate is colored. Three Li atoms directly connected to an oxygen atom of the colored enolate unit are colored orange. (b) Schematic view of an enolate unit, indicating axial chirality.

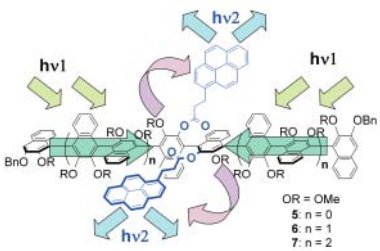
Stereochemical Reversal in Asymmetric Cyclization: Enolate Chemistry at Room Temperature



Treatment of an amino acid derivative **3** by potassium hexamethyldisilazide (KHMDS) in DMF at −60°C gave (*S*)-**4** in 98% ee, while that by KOH in DMSO at room temperature gave (*S*)-**4** even in higher enantioselectivity (99% ee). This could be ascribed to the enhanced reactivity of an amine-free potassium enolate generated by KOH in DMSO. Contrary to this process, treatment of **3** with lithium 2,2,6,6-tetramethylpiperidide (LTMP) in THF at room temperature gave (*R*)-**4** in inversion of the configuration in 91% ee. Interestingly, the similar treatment of **3** with LTMP at −60°C gave (*R*)-**4** in much lower enantioselectivity (41% ee).

Optical Properties of Oligo(2,3-dioxyfunctionalized)naphthalenes

A series of oligo(2,3-dioxyfunctionalized)naphthalenes **5-7** that possess two pyrene groups on the central scaffolding oxygen functions are synthesized. When the naphthalene units are selectively exited at 310 nm, the fluorescence from the pyrene units was observed. This result demonstrates that an effective intramolecular energy transfer occurs from the naphthalene units to the pyrene units. The intramolecular energy transfer quantum yields of **5-7** were around 20% regardless of the number of naphthalene units. Thus, the optical properties of oligonaphthalenes are more than sum of the discrete naphthalene units. These properties are expected to be produced by coupling the transition moments that run parallel to the minor axis of the naphthalene ring.



Scientific Research (B) (2), 1 April 2002 - 31 March 2005.

Awards

Tanima D, Best Poster Award, 11th Summer Meeting of Functional Host-Guest Chemistry (Toyama), 28 July 2005.

Monguchi D, Best Poster Award, 25th Seminar on Synthetic Organic Chemistry for Young Scientists, 24 November 2005.

Takaishi K, Best Poster Award, 25th Seminar on Synthetic Organic Chemistry for Young Scientists, 24 November 2005.

Division of Synthetic Chemistry
- Advanced Inorganic Synthesis -

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

Prof
SHIMAKAWA, Yuichi
(D Sc)

Assoc Prof
AZUMA, Masaki
(D Sc)

Assist Prof
IKEDA, Yasunori

A Res
MASUNO, Atsunobu
(D Sc)

Students

KAWAI, Masanori (M1)
SAKAI, Maiko (M1)
NAKAMURA, Motonori (RF)

Visitors

Prof POEPPELMEIER, Kenneth R. Northwestern University, USA, 16-17 March 2005
Prof SALJE, Ekhard K.H. Cambridge University, UK, 15 September 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Current-Induced Electroresistive Effect in Microfabricatied Perovskite Manganite thin films, Masuno A, Terashima T, Shimakawa Y, Takano M, Spring Meeting of Japan Society of Powder and Powder Metallurgy, Tokyo Japan, 1 June 2005.

A Designed New Ferromagnetic Ferroelectric Bi_2NiMnO_6, Azuma M, Takata K, Shimakawa Y, Takano M, Joint 20th AIRAPT-43rd EHPRG Conference on Science and Technology of High Pressure, Karlsruhe, Germany, 28 June 2005.

Search for New Functional Materials under Ultra High Pressure, Azuma M, 2005 Autumn Meeting of Physical Society of Japan, Kyoto, Japan, 20 September 2005.

New Ferromagnetic Ferroelectric Oxide with Double Perovskite Structure, Shimakawa Y, 2005 Autumn Annual Meeting of Japan Institute of Metals, Hiroshima, Japan, 29 September 2005.

New Ferromagnetic Ferroelectric Bi_2NiMnO_6 Compound with Double-Perovskite Structure, Shimakawa Y, Azuma M, Takata K, Hashisaka M, Kan D, Masuno A, Sakai M, Terashima T, Mibu K, Takano M, 12th US-Japan Seminar on Dielectric and Piezoelectric Ceramics, Annapolis, U.S.A., 8 November 2005.

Thermal Stability of $BaTi_2O_5$ Phase, Ikeda Y, Takata K, Shimakawa Y, Asaoka Y, Takada J, Kusano Y, Fall Meeting of Japan Society of Powder and Powder Metallurgy, Shizuoka, Japan, 16 November 2005.

Grants

Shimakawa Y, Collaboratory on Electron Correlations –Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2004 - 31 March 2006.

Shimakawa Y, Invention of Anormalous Quantum Materials –New Physics through Innovative Materials– Scientific Research on Priority Areas, 1 April 2005 - 31 March 2007.

Azuma, M, Search for Ferromagnetic Ferroelectrics in Lead, Bismuth-3*d* Transition Metal Double Perovskites with Controlled Arrangements of Elements, Natural Sciences Research Assistance, The Asahi Glass Foundation, 1 April 2005 - 31 March 2007.

Single-layer Oxychloride Superconductor $Ca_{2-x}CuO_2Cl_2$ with A-site Cation Deficiency

Superconductivity in copper oxides occurs when adequate numbers of hole or electron carriers are introduced into an antiferromagnetic insulator with CuO_2 planes. Copper oxychloride $Ca_2CuO_2Cl_2$ shown in fig. 1(a) has a single CuO_2 plane, the same as La_2CuO_4. Hole doping by substituting Na for Ca to make this compound superconducting was accomplished using high-pressure (HP) synthesis at 6 GPa. $Ca_{2-x}Na_xCuO_2Cl_2$ has the highest T_C=28 K at x=0.20. The ease of sample preparation with a lightly hole-doped composition, an absence of structural changes at low temperature, an absence of structural modulation, and excellent single crystal sample cleavage are ideal for surface sensitive measurements. Investigations into this compound's electronic state using angle-resolved photoemission spectroscopy and scanning tunneling microscopy/spectroscopy are attracting great attention.

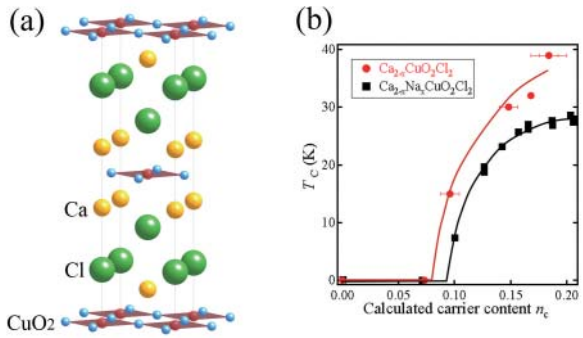


Figure 1. (a) Crystal structure of $Ca_2CuO_2Cl_2$. (b) Carrier number dependence of T_C in $Ca_{2-x}CuO_2Cl_2$ and $Ca_{2-x}Na_xCuO_2Cl_2$.

We have found new oxychloride superconductor $Ca_{2-x}CuO_2Cl_2$ without cation substitution by using high-pressure synthesis. The highest T_C was 38 K, 10 K higher than that of $Ca_{2-x}Na_xCuO_2Cl_2$. Structure analysis based on synchrotron x-ray and neutron powder diffractions revealed that the Ca deficiency was the origin of the hole carrier. This compound has two structural features as compared to $Ca_{2-x}Na_xCuO_2Cl_2$; fewer defects and a shorter Cu-Cl bond length. Postannealing at 773 K led to a further increase of the T_C to 43 K. This superconductor with a flat CuO_2 plane might form the basis for future discussions about the factors that determine the T_C of single-layer cuprates.

I. Yamada et al., *Phys. Rev. B*, **72**, 224503 (2005).

Pressure/Temperature/Substitution-induced Melting of *A*-site Charge Disproportionation in $Bi_{1-x}La_xNiO_3$ $0 \leq x \leq 0.5$

Charge ordering is a common phenomenon in mixedvalence transition-metal oxides, but it attracts much attention because of competition with fascinating metallic behavior exhibiting superconductivity or giant magnetoresistance. The competition between them has been keenly discussed as a clue for understanding the origin of such striking properties. In addition to the mixed-valence systems, several integer-valence perovskite oxides such as $CaFeO_3$ and $ANiO_3$ (A=Y, Pr, Nd...) also show a charge-ordering transition described as $2M^{n+} \rightarrow M^{(n-\delta)+} + M^{(n+\delta)+}$, which is called charge disproportionation (CD).

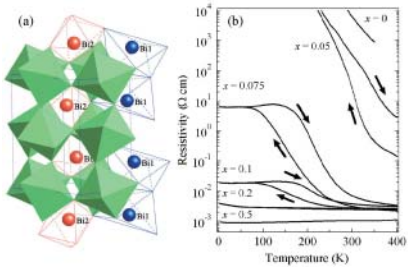


Figure 2. (a) Crystal structure of $BiNiO_3$. (b) Temperature dependence of resistivity of $Bi_{1-x}La_xNiO_3$.

$BiNiO_3$ (x=0) is a triclinic perovskite with a unique valence state of $Bi^{3+}{}_{0.5}Bi^{5+}{}_{0.5}Ni^{2+}O_3$. This is the only known compound with A-site charge disproportionation. Synchrotron x-ray powder diffraction revealed that pressure (P~3 GPa, T=300 K), temperature (T~340 K, x=0.05), and La substitution (x=0.075, T=300 K) caused the structural change from a triclinic insulating to an orthorhombic metallic symmetry, suggesting melting of the A-site charge disproportionation. Comparing crystal structure and physical properties with the other $ANiO_3$ series, an electronic state of the metallic phase can be described as $A^{3+}\underline{L}$, $Ni^{2+}\underline{L}$, where a ligand-hole L contributes to a conductivity.

S. Ishiwata et al., *Phys. Rev. B* **72**, 045104 (2005).

Figure 3. Image of "Collaboratory" on neutron diffraction studies. Real-time data sharing and video-meeting between KEK, Tsukuba and ICR, Uji.

Awards

Azuma M, Young Scientists' Prize, the Commendation for Science and Technology by the MEXT, 20 April 2005.

Ikeda Y, The L'Oréal Art & Science of Color prizes, 21 October 2005.

Division of Materials Chemistry
- Chemistry of Polymer Materials -

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

Prof
FUKUDA, Takeshi
(D Eng)

Assoc Prof
TSUJII, Yoshinobu
(D Eng)

Assist Prof
OHNO, Kohji
(D Eng)

Assist Prof
GOTO, Atsushi
(D Eng)

PD
GAO, Weiping
(Ph D)

PD
ARITA, Toshihiko
(D Sc)

Students

MORINAGA, Takashi (D3)
YOSHIKAWA, Chiaki (D3)
KWAK, Yungwan (D3)
OMI, Yohei (M2)
OKAYASU, Kenji (M2)
ZUSHI, Hirokazu (M2)
TAKENO, Satoshi (M2)
KURAMOTO, Mamoru (M1)
TAI, Yugo (M1)
TEZUKA, Miho (M1)
TABATA, Hiroshi (UG)
HIRAI, Norihiro (UG)

Visitors

Prof RUSSELL, Gregory T.	University of Canterbury, New Zealand, 12 April 2005
Prof BUBACK, Michael	University of Göttingen, Germany, 19 August 2005
Dr VANA, Philipp	University of Göttingen, Germany, 1 - 30 November 2005
Prof MATYJASZEWSKI, Krzysztof	Carnegie Mellon University, USA, 17 November 2005
Prof KISHIDA, Akio	Tokyo Medical and Dental University, Tokyo, 26 November 2005
Dr ALDABBAGH, Fawaz	National University of Ireland, Ireland, 5 December 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Surface Interactions of CPB (Invited Lecture), Tsujii Y, and 1 other presentation, 3rd KIPS-NIST Symposium on Polymer Science, Kyoto, 19 - 20 May.

5 presentations, 54th Spring Meeting, Soc. Polym. Sci., Jpn., Yokohama, 25 - 27 May.

Structure and Properties of CPB (Invited Lecture), Tsujii Y, Workshop on Organized Macromolecular Systems, Fukuoka, 29 July.

Surface-initiated LRP and CPB: Their Unique and Striking Properties (Invited Lecture), Fukuda T, and 4 other presentations, 230th ACS Fall 2005 National Meeting, Washington DC, USA, 28 Aug - 1 September.

5 presentations, 54th Autumn Meeting, Soc. Polym. Sci., Jpn., Yamagata, 20 - 22 September.

Science for New Surface -CPB- (Invited Lecture), Fukuda T, Frontier Symposium on Polymer Science, Yamagata, 20 September.

Science and Technology of CPB, Fukuda T, and 7 other presentations, Symposium on CPB, ICR, 26 November.

Surface with CPB: Their Unique and Striking Properties (Invited Lecture), Fukuda T, and 3 other presentations, Pacifichem 2005 International Chemical Congress, Honolulu, USA, 15 - 20 December.

Synthesis of Monodisperse Silica Particles Coated with Well-Defined, Concentrated Brushes by Surface-Initiated Atom Transfer Radical Polymerization

Monodisperse silica particles (SiPs) of diameter between 100 and 1500 nm were surface-modified in a mixture of ethanol/water/ammonia with a newly designed triethoxysilane having an atom transfer radical polymerization (ATRP) initiating site, (2-bromo-2-methyl)propionyloxyhexyl triethoxysilane. The surface-initiated ATRP of methyl methacrylate (MMA) mediated by a copper complex was carried out with the initiator-fixed SiPs in the presence of a "sacrificial" (free) initiator. The polymerization proceeded in a living manner in all examined cases, producing SiPs coated with well-defined PMMA of a target molecular weight up to 480 k with a graft density as high as 0.65 chains/nm^2. These hybrid particles had an exceptionally good dispersibility in organic solvents. Transmission electron microscopic and atomic force microscopic observations of their monolayers prepared at the air-water interface revealed that they formed an ordered 2-dimensional lattice extending throughout the monolayer (Figure 1).

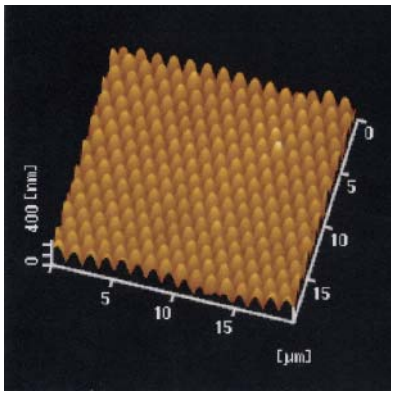


Figure 1. Ordered 2-dimensional lattice of monodisperse silica particles coated with well-defined, concentrated brushes.

Protein Repellency of Well-Defined, Concentrated Poly(2-hydroxyethyl methacrylate) Brushes by Size-Exclusion Effect

The adsorption of proteins on poly(2-hydroxyethyl methacrylate) (PHEMA) brushes was systematically studied by quartz crystal microbalance (QCM) (Figure 2) and fluorescence microscopy as a function of graft density and protein size. The graft density σ (chains/nm^2) ranged from 0.007 (dilute or semi-dilute brush regime) to 0.7 (concentrated brush regime), and the protein size ranged from 2 to 13 nm in an effective diameter. The lowest-density brush (σ = 0.007) adsorbed all the tested four proteins, while the highest-density brush (σ = 0.7) adsorbed none of them. The middle-density brush (σ = 0.06) showed an intermediate behavior, adsorbing the smallest two proteins but effectively repelling the largest two. These results support the idea of size-exclusion effect, an effect characteristic of concentrated polymer brushes, in which the graft chains are highly extended and highly oriented so that large molecules, sufficiently large compared with the distance between the nearest-neighbor graft points, are *physically* excluded from the entire brush layer.

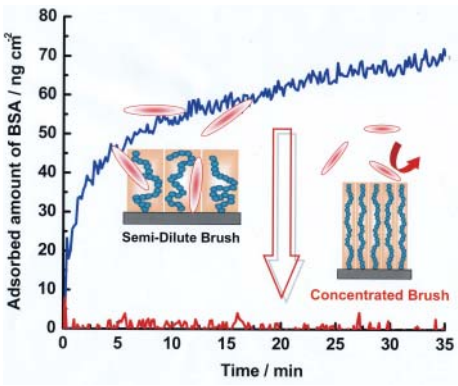


Figure 2. Adsorption of bovine serum albumin (BSA) on PHEMA brushes.

Grants

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

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

Tsujii Y, Patterning by Direct-Writing Graft Polymerization, Grant-in-Aid for Exploratory Research, 1 April 2005 - 31 March 2007.

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

Ohno K, Fundamentals and Applications of Semi-Soft Colloidal Crystals, Industrial Technology Research Grant Program by NEDO, 1 January 2005 - 31 December 2007.

Tanaka K, Construction of Nanoelectronic Devices, CREST, Jpn. Sci. Tech. Corp., 1 November 2002 - 31 October 2007.

Kaya K, Collaboratory on Electron Correlations, Grant-in-Aid for Cre. Sci. Res., 1 April 2001 - 31 March 2006.

Award

Tsujii Y, The Award of the Society of Fiber Science and Technology, Studies on Precise Surface Modification by LRP, The Society of Fiber Science and Technology, Japan, 8 July 2005.

Division of Materials Chemistry
- Chemistry of Polymeric Functionality Materials -

http://www.scl.kyoto-u.ac.jp/~kohjshin/index.htm

Prof
KOHJIYA, Shinzo
(D Eng)

Assoc Prof
TSUJI, Masaki
(D Eng)

Assist Prof
TOSAKA, Masatoshi
(D Eng)

Assist Prof
SENOO, Kazunobu
(D Eng)

A Res
YOSHIOKA, Taiyo
(D Eng)

Students

NAKAO, Toshio (D3)
POOMPRADUB, Sirilux (D3)
KAWAKAMI, Daisuke (M2)
MATSUDA, Shota (M2)
FUJIMURA, Takashi (M2)
TAKAHASHI, Ryosuke (M1)
TOGAI, Manabu (M1)
MURACHI, Yuki (M1)
KAN-NAN, Haruhisa (UG)
HAYAKAWA, Yoshinori (UG)
KOBAYASHI, Keisuke (UG)

Visitors

Dr KRACOVSKY, Ivan	Charles University, Czech Republic, 30 August 2004 - 26 August 2005
Dr MAGONOV, Sergei	Digital Instruments/Veeco, USA, 15 July 2005
Dr LIZ-MARZÁN, Luis M	University of Vigo, Spain, 26 July 2005

Scope of Research

Relationships between molecular arrangements in polymeric functionality materials and their properties are investigated. Formation mechanisms of higher order structures are elucidated by electron microscopy and X-ray diffraction measurements. The major research subjects are as follows: (1) Strained-induced crystallization of natural rubber, (2) Ionic conductivity of uniaxially stretched elastomer, (3) Direct observation of molecular chains in the epitaxially grown lamellar crystals of polymers, (4) Polymer gel consisting of the stereoregular polystyrene and (5) Spontaneous nano-scale patterning on uniaxially oriented polymer layers.

Research Activities (Year 2005)

Presentations

"Three-Dimensional Dispersion of Nano-Fillers in Soft Nano-Composite as Revealed by 3D-TEM / Electron Tomography", Kohjiya S, Materials 2005, 7th Portuguese Materials Society Meeting, 3rd International Materials Symposium, Aveiro, Portugal, 20 - 23 March.

"Smart Nano-Composite: Strain-Induced Crystallization of Natural Rubber", Kohjiya S, 10th International Seminar on Elastomers, Rio de Janeiro, Brasil, 5 - 8 April.

"Nano-Structural Elucidation in Carbon Black Loaded NR Vulcanizate by 3D-TEM and In Situ WAXD Measurements", Kohjiya S, Kato A, Shimanuki J, Ikeda Y, Tosaka M, Poompradub S, Toki S, Hsiao B S, Spring 167th Technical Meeting of the Rubber Division, ACS, San Antonio, Texas, USA, 16 - 18 May, and other 1 presentation.

"Morphological Study on Uniaxially Oriented Thin Films of Polyesters", Yoshioka T, Fujimura T, Tsuji M, Kohjiya S, Kawahara Y, 54th SPSJ Annual Meeting, Yokohama, Japan, 25 - 27 May, and other 11 presentations.

"Dynamical Study on Strain-Induced Crystallization of Natural Rubber Networks: Behavior as a Smart Nanocomposite", Kohjiya S, 5th International Symposium Molecular Mobility and Order in Polymer Systems, St. Petersburg, USA, 20 - 24 June.

"Physical Gelation of Syndiotactic Polystyrene in the Presence of Poly(Ethylene Oxide)", Senoo K, Matsuda S, Kohjiya S, The International Rubber Conference 2005 Yokohama, Yokohama, Japan, 24 - 28 October.

Grants

Kohjiya S, Stress-Induced Crystallization Behavior of Natural Rubber, Grant-in-Aid for Scientific Research, (B) (2), 1 April 2003 - 31 March 2005.

Tsuji M, High-resolution TEM of the Shish-Kebab Structure in Uniaxially Oriented Polyesters, Grant-in-Aid for Scientific Research, (C) (2), 1 April 2004 - 31 March 2007.

Morphological Study on Uniaxially Oriented Thin Films of PBT

The molecular weight of aromatic polyesters falls off easily in the molten state, mostly due to the transesterification reaction. Accordingly, the formation of the shish-kebab structure consisting of central extended-chain crystal and folded-chain crystals has been considered to be fairly difficult. We prepared uniaxially oriented thin films of poly(butylene terephthalate) (PBT), one of aromatic polyesters, by applying shear strain to the melt and studied their resulting morphology by transmission electron microscopy. Formation of stacked-lamellar structures in this aromatic polyester was visually evidenced. On the basis of crystallographic consideration, we assigned each of the recognized stacked-lamellar structures to a shish-kebab structure or a part of it. In addition, we successfully demonstrated that, in one shish-kebab structure, all or almost all kebabs (namely, lamellae) have a same crystallographic orientation. Fig. 1 is a set of dark-field images obtained from the same specimen region. In the left side (untilted) image, no remarkable morphology is recognized, while in the right side image tilted by 15°, some stacked-lamellar structures are observed. This change in appearance of the stacked lamellar structures, depending on the direction of the incident electron beam, suggests that all of the lamellae in one observed group as a stacked-lamellar structure have a same crystallographic orientation against the direction of incident electron beam.

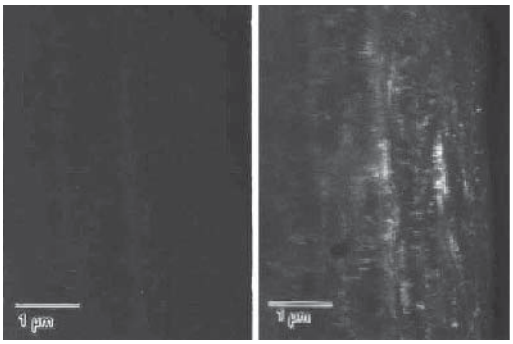


Figure 1. Dark-field images of PBT taken from the same specimen area: (left) un-tilted and (right) tilted by 15° around the vertical axis (shearing direction). Both images were taken mainly by using a 100 reflection of the α form. The shearing direction is vertical.

Self-Assembly of Nano-Sized Arrays on Highly Oriented Thin Films of Poly(Tetrafluoroethylene)

Self-assembly of nano-sized arrays by casting a dilute solution of a guest material on the friction-transferred poly(tetrafluoroethylene) (FT-PTFE) substrate was newly discovered. Long axis of the rod-like structures forming the arrays is aligned perpendicular to the chain direction of FT-PTFE, and accordingly, the arrays are highly anisotropic. This phenomenon was observed for aqueous or organic solutions of polymers or organic materials. The arrays in question are formed regardless to the crystallinity of the guest materials. The formation mechanism of the nano-sized arrays is still unclear. However, we guess that they are formed as a result of microscopic flow pattern at the edge of the solution film, according to the observation of the dynamic structure in the drying solution by optical microscopy. The arrays in question may be a new type of dissipative structure. If formation of the nano-sized arrays can be controlled, this phenomenon may be applicable to fabrication of, e.g., optical devices.

Figure 2. Nano-sized arrays prepared from atactic polystyrene. Scale bar is 500 nm. The molecular chains of PTFE are oriented vertically.

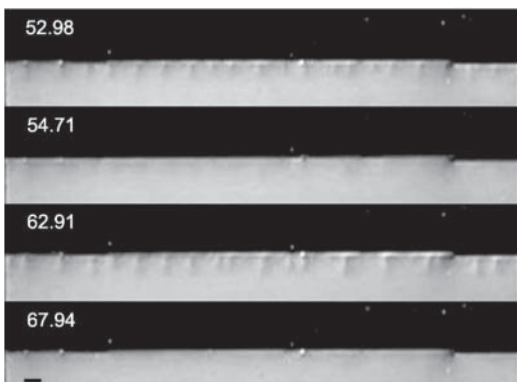


Figure 3. Time series of a drying film of a dilute solution of atactic polystyrene. Elapsed time (sec) is indicated at the left side of each part. The FT-PTFE / glass surface is exposed in the upper dark area, while the lower bright area is covered by the solution. The molecular chains of PTFE are oriented horizontally. Scale bar is 10 μm.

Division of Materials Chemistry
- Inorganic Photonics Materials -

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

Prof
YOKO, Toshinobu
(D Eng)

Assoc Prof
TAKAHASHI, Masahide
(D Sc)

Assist Prof
TOKUDA, Yomei
(D Eng)

A Res
MENAA, Bouzid
(Ph D)

PD
KANG, Eun-Seok
(Ph D)

Students

MIZUNO, Megumi (D3)
OHTANI, Shoichi (M2)
MAEDA, Takahiro (M2)
MIYAMOTO, Ayako (M2)
KOUNO, Ryo (M1)
MATSUDA, Kazuomi (M1)
SUZUKI, Masaru (M1)
FUJII, Masao (UG)
UEMURA, Kouji (UG)
YAMAMOTO, Hideaki (UG)
FUKUDA, Masahiro (RF)
FUKUDA, Masaaki (RF)
KUNIYOSHI, Minoru (RF)
TOMOYOSHI, Yoshio (RF)
NAKATA, Kunihiko (RF)

Visitors

Prof INNOCENZI, Plinio — University of Sassari, Italy, 17 January - 14 February 2005
Prof BABONNEAU, Florence — Université Paris 6, France, 7 November 2005
Prof BONHOMME, Christian — Université Paris 6, France, 7 November 2005

Scope of Research

In this laboratory, amorphous and polycrystalline inorganic materials and organic-inorganic hybrid materials with various optical functions such as photorefractivity, optical nonlinearity and photocatalysis are the target materials, which are synthesized by sol-gel, multi-cathode sputtering, melt-quenching and sintering methods and so on. Aiming at highly functional materials the structures are investigated by X-ray diffraction techniques, high-resoluction NMR, thermal analysis, various laser spectroscopies and ab initio molecular orbital calculations.

Research Activities (Year 2005)

Presentations

Optical Characteristics of Organic-inorganic Hybrid Material Derived Through Non-hydrolytic Reaction and Photo-Polymerization, Kang E., Takahashi M., Yoko T., The 105th Annual Meeting the American Ceramics Society, Baltimore, 15 - 17 April.

Preparation and NLO Properties of Dye-doped Polysiloxane-based Glass Thick Films, Menaa B., Takahashi M., Mizuno M., Tokuda Y., Yoko T., MC7: Functional Materials for the 21st Century, Edinburgh (UK), 6 - 9 July.

Organic-inorganic Hybrid Materials Prepared through Non-aqueous Acid-base Reactions, Takahashi M., Mizuno M., Kakiuchida H., Menaa B., Tokuda Y., Yoko T., 13th International Workshop on Sol-gel Science and Technology (Sol-gel2005), Los Angels, USA, 21 - 26 September.

Optical Characteristics of Organic-inorganic Hybrid Material Derived through Non-hydrolytic Reaction and Photo-polymerization, Kang E., Takahashi M., Yoko T., 6th Pacificrim Conference on Ceramics and Glass Technology, Maui, Hawaii, USA, 16 September.

Grants

Yoko T., Preparation of Organic-inorganic Hybrid Low-melting Glasses through Acid-base Reaction, Asahi Glass Foundation, 1 April 2004 - 31 March 2005.

Takahashi M., Inhomogeneous Structures in the Glasses, Grant-in-Aid for Scientific Research for Encouragement of Young Scientists (A), 1 April 2004 - 31 March 2006.

Takahashi M., Development of Photonics Materials Based on the Organic-inorganic Hybrid Low Melting Glasses, PRESTO, Japan Science and Technology Agency, 1 November 2002 - 31 March 2006.

Takahashi M., Organic-inorganic Hybrid Low-melting Glasses Doped with Optical Active Centers via Non-aqueous Acid-base Reaction, Murata Scientific Foundation, 1 July 2004 - 31 June 2005.

Takahashi M., Fabrication of Large Area Photonic Films, Toyota Physical & Chemical Research Institute, 1 April

Fabrication of Periodic Photonic Structure of TiO_2 and Other Oxides on Sol-gel Dip Coated Films through Photo-Polymerization Induced Phase Separation (PIPS)

By combining PIPS with sol-gel coating technique, we can obtain photonic structures shown in Fig. 1. Pictures show the TiO_2 phase grating obtained by holographic illumination of Ar^+-ion laser light (inset shows the SEM image of the obtained gratings). The periodicity could be controlled in the range from 500 nm to 20 μm depending on the holographic condition of irradiated laser light. When the PIPS and sol-gel conditions are appropriately controlled, we can fabricate periodic structure without laser (coherent) light source. Fig. 2 shows an AFM image of the TiO_2 2D-photonic structure obtained by the present method using a black light as UV source. The 2D structure is self-organized on the substrate. This method has a great advantage compared to the photo-polymerization method of vinyl-modified metal alkoxides system. With complete condensation, a large value of Δn is expected.

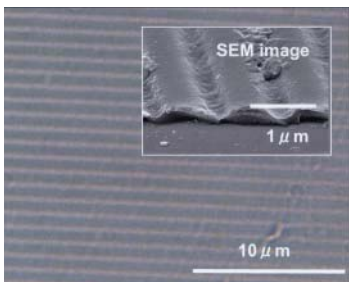


Figure 1. Titania phase grating obtained by PIPS in combination with the sol-gel coating technique. Inset shows the SEM image of fractured edge of the obtained grating.

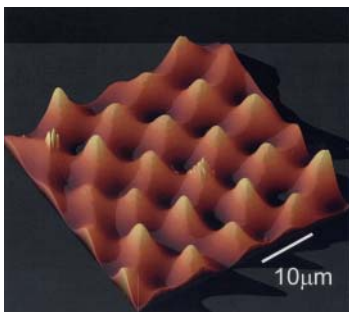


Figure 2. 2D photonic structure of TiO_2 obtained by irradiating a black light. The periodic structure was obtained by controlling PIPS conditions.

Structural Study on Organically-Modified Polysiloxane Glasses

We have already reported that low-melting glass can be prepared using a gel derived by the sol-gel method. The glasses with compositions of $xPh_2SiO_{2/2}$-$(1-x)PhSiO_{3/2}$ ($0 < x \leq 30$) were prepared and their softening temperatures are widely dispersed around 150°C. In order to examine factors affecting the softening behavior, structural study has been performed using ^{29}Si MAS NMR (Magic Angle Spinning Nuclear Magnetic Resonance) spectroscopy and GPC (Gel Permeation Chromatography) measurements. First, we obtained the frequency at G" (the imaginary part of the elastic modulus) = 10^3 Pa using viscoelastic measurements. Second, we acquired the condensation degree of Si, <m>, which is the number of Si-O-Si bonding per one Si by NMR spectra and the molecular volume, <M>, by GPC measurements. Finally, we have found a relation between the frequency at G"=10^3 Pa, the condensation-degree and molecular volume as follows,

$$\log\omega_{G''=10^3 Pa} = -9.2\langle m\rangle - 5.0\log\langle M\rangle + const.$$

We have also found that the rate of increase in elastic modulus induced by heat-treatment decreases with increasing amount of $Ph_2SiO_{2/2}$ unit.

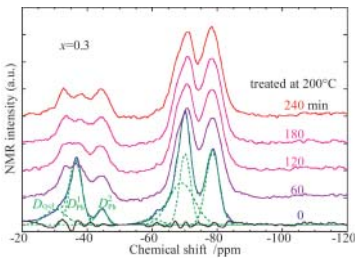


Figure 3a. ^{29}Si MAS NMR spectra of $xPh_2SiO_{2/2}$-$(1-x)PhSiO_{3/2}$ glasses. Numericals represent the heat-treatment time.

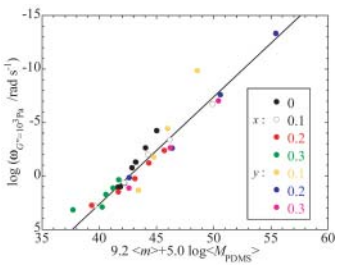


Figure 3b. A relationship between the frequency at G" =10^3 Pa, the condensation-degree and molecular volume for $xPh_2SiO_{2/2}$-$(1-x)PhSiO_{3/2}$ glasses.

2005 - 31 March 2006.

Kakiuchida H., Softening Behavior of Organic-inorganic Hybrid Glasses and its Application for Photonic Devices, ICR Grants for Young Scientists.

Awards

6th Pacificrim Conference on Ceramics and Glass Technology, Student Poster Award, "Fabrication of TiO_2 Periodic Structure by the Photopolymerization-induced Phase Separation Method", Maeda T., Takahashi M., Yao J., Tokuda Y., Nishii J. and Yoko T., 6th Pacific Rim Conference on Ceramic and Glass Technology, 11 - 16 September 2005.

BCSJ Paper Award, "Conducting and Magnetic Properties of 1-Ethyl-3-methylimidazolium (EMI) Salts Containing Paramagnetic Irons: Liquids $[EMI][M^{III}Cl_4]$ (M = Fe and $Fe_{0.5}Ga_{0.5}$) and Solid $[EMI]_2[Fe^{II}Cl_4]$", Yoshida Y., Otsuka A., Saito G., Natsume S., Nishibori E., Takata M., Sakata M., Takahashi M., and Yoko T.

Division of Materials Chemistry
- Magnetic Materials -

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

Prof
ONO, Teruo
(D Sc)

Assoc Prof
KOBAYASHI, Kensuke
(D Sc)

Assist Prof
KASAI, Shinya
(D Sc)

Assist Prof (NEDO)
YAMAGUCHI, Akinobu
(D Sc)

Techn
KUSUDA, Toshiyuki

Students

OOKOUCHI, Takuo (D3)
JIKO, Norihiro (D3)
HIMENO, Atsushi (D2)
TANIGAWA, Hironobu (M2)
MORIMOTO, Yasumasa (M2)
WATANABE, Shinichi (M2)
DELMO, Michael Picazo (M1)
TAMADA, Yoshinori (M1)
YANO, Kuniaki (M1)

Visitors

Prof HILLEBRANDS, Burkard	Technische Universitaet Kaiserslautern, Germany, 11 April 2005
Dr PARKIN, Stuart	IBM Almaden Research Center, USA, 14 June 2005
Prof AHARONY, Amnon	Tel Aviv University, Israel, 24 October 2005
Prof ENTIN-WOHLMAN, Ora	Tel Aviv University, Israel, 24 October 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Thermal Effect on Current-driven Domain Wall Motion in Magnetic Nanowires, Yamaguchi A, Nasu S, Tanigawa H, Ono T, Workshop on Thermally Assisted MRAM and Thermo-magnetics, 9 April 2005, Nagoya, Japan.

Depth-Profile of Spin Polarization in Nonmagnetic Layers of Epiaxial Fe/Au(001) Multilayers by Resonant X-ray Magnetic Scattering, Ohkochi T, Mibu K, Hosoito H, Otsuka Y, Kodama K, Kasai S, Ono T, 50th Magnetism and Magnetic Materials Conference, 30 October-3 November 2005, San Jose, California, USA.

Ratchet Effect of a Magnetic Domain Wall in Asymmetric Magnetic Wires, Himeno A, Kasai S, Ono T, 50th Magnetism and Magnetic Materials Conference, 30 October-3 November 2005, San Jose, California, USA.

Domain Wall Resistance in FePt Wire with Perpendicular Magnetic Anisotropy, Tanigawa H, Yamaguchi A, Kasai S, Ono T, Seki T, Shima T and Takanashi K, 50th Magnetism and Magnetic Materials Conference, 30 October-3 November 2005, San Jose, California, USA.

Reduction of the Threshold Current Density for the Current-driven Domain Wall Motion by Shape Control, Yamaguchi A, Tanigawa H, Yano K, Kasai S, and Ono T, 50th Magnetism and Magnetic Materials Conference, 30 October-3 November 2005, San Jose, California, USA.

Spin Structures of Chromium in Epitaxial Multilayers Cr(001)/X (X=Sn, Au, V), Jiko N, Otsuka Y, Mibu K, Takeda M, 50th Magnetism and Magnetic Materials Conference, 30 October-3 November 2005, San Jose, California, USA.

Grants

Ono T, Control of Physical Properties by Utilizing Spin-Polarized Current, Grant-in-Aid for Scientific Research (A), 1 April 2005 - 31 March 2008.

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

Synthesis of the World's Smallest Magnets

Arrays of monodisperse FePt nanocrystals in the $L1_0$ structure are excellent candidates for future recording media with ultrahigh densities beyond 1 Tb/in^2. We successfully synthesized monodisperse $L1_0$-FePt nanocrystals that are not only superior in magnetism but also easy to handle through being dispersible in solvents. Although the thermal treatment is necessary to form the ferromagnetic $L1_0$ structure, this process induces coalescence and coarsening of nanocrystals and previously made it challenging to obtain particulate $L1_0$-FePt. We have solved this problem by coating nanocrystals with thick SiO_2, which allows thermal treatment even at 900°C. The protecting shell was thereafter removed in a specific way that enabled us to recover the $L1_0$-FePt nanocrystals in water dispersion. The SiO_2-coated nanocrystals show a high coercivity up to 18.5 kOe at room temperature in spite of their core size of only 6.5 nm in diameter. Thus, the resultant nanocrystal is the smallest magnet that is stable at room temperature and one of the most promising materials for the near-future recording media. We also demonstrated that the solvent-dispersed $L1_0$-FePt nanocrystals orient their magnetic and structural axis along an external magnetic field.

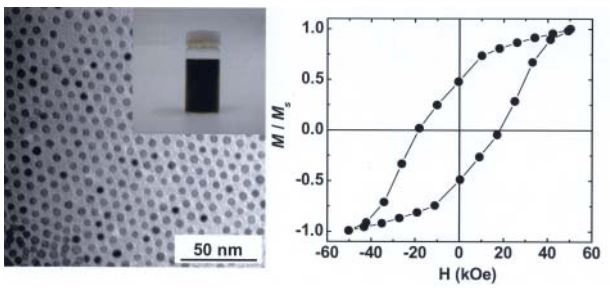


Figure 1. TEM image of the $L1_0$-FePt nanocrystals. Insetshows an image of the solution containing the nanocrystals (right). Room-temperature hysteresis loop in the magnetization of the nanocrystals (left).

Ratchet Effect of the Domain Wall in Asymmetric Magnetic Wires

Magnetic domain wall (DW) motion in submicron wires can be activated not only by applying a magnetic field but also by passing an electric current through the wire. Our discovery of the current-driven DW motion has opened up very interesting perspectives for using manipulated DWs in magnetic memory and logic devices. We have extended our research to the current-driven DW motion in magnetic wires with asymmetric notches. It was found that the critical current density necessary for the current-driven DW motion depends on the propagation direction of the DW, and that the DW moves more easily in the direction along which the slope of the asymmetric notch is less inclined. In other words, the asymmetric notch works as an asymmetric potential for the current-driven DW motion (see the top panel of Fig. 2). This phenomenon may be called as a "*magnetic ratchet effect*". The middle panel of Fig.2 shows the relation between the critical current density and the applied magnetic field. Red and blue dots show the current density for the rightward and the leftward propagation, respectively. The inclinations of the two lines of the magnetic field dependence of the current density are different between the propagation directions of the DW (see the bottom panel of Fig.2), which supports the asymmetric potential due to the asymmetric notches.

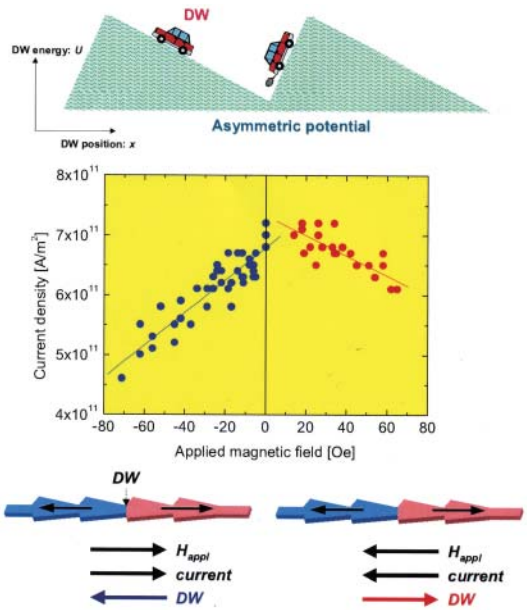


Figure 2. Schematic illustration of the motion of magnetic domain wall in asymmetric potential barriers (top). Magnetic field dependence the critical current density (middle). Red and blue dots show the values of the critical current density for the rightward and the leftward propagation, respectively. The magnetic stucture and the directions of a current and a magnetic field are shown (bottom).

Ono T, Development of Writing Technology for Gbit-MRAM by Using Current-driven Domain Wall Motion, Industrial Technology Research Grant Program from NEDO, 1 January 2005 - 31 December 2007.

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

Award

Ono T, Marubun Academic Award, Marubun Research Promotion Foundation, 7 March 2005.

Division of Biochemistry
- Biofunctional Design-Chemistry -

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

Prof
FUTAKI, Shiroh
(D Pharm Sc)

Assist Prof
IMANISHI, Miki
(D Pharm Sc)

PD
NINOMIYA, Keiko
(D Sc)

PD
TADOKORO, Akiko
(D Sc)

Students

SHIRAISHI, Yasuhisa (D3)
YAN, Wei (D1)
TAKEUCHI, Toshihide (D1)
KAWABATA, Noriko (M2)
SONOMURA, Kazuhiro (M2)
HIGASHI, Chika (M2)
KOSUGE, Michie (M1)
MORISAKI, Tatsuya (M1)
SASAZAKI, Toshimasa (UG)

Visitors

Prof MEZO, Gabor — Hungarian Academy of Sciences, Hungary, 24 - 26 October 2005
Prof FUDECZ, Ferenc — Hungarian Academy of Sciences, Hungary, 25 - 26 October 2005
Mr BANOCZI, Zoltan — Hungarian Academy of Sciences, Hungary, 11 July - 13 August 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

"Cell-penetrating Peptides and Applications" Futaki S, Wenner-Gren Foundations International Symposium, Stockholm, Sweden, 19 May.

"Control of Peptide Structure and Function by Fe(III)-Induced Helix Destabilization" Futaki S, Kiwada T, Sugiura Y, 19th American Peptide Symposium, San Diego, USA, 18 - 23 June.

"Effect of Counteranions and Membrane Potential on the Cellular Uptake of Arginine-rich Peptides" Takeuchi T, Nakase I, Sugiura Y, Sakai N, Matile S, Futaki S, 19th American Peptide Symposium, San Diego, USA, 18 - 23 June.

"Artificial 6-zinc Finger Peptides with Various Linkers" Imanishi M, Sugiura Y, Metalloprotein and Protein Design Conference, Chicago, USA, 30 July.

"Counteranion-Mediated Delivery of Arginine-Rich Peptides into Living Cells" Takeuchi T, Kosuge M, Tadokoro A, Sugiura Y, Nishi M, Kawata M, Sakai N, Matile S, Futaki S, 42th Japanese Peptide Symposium, Suita, 28 October.

"The Effect of Octaarginine on the Translocation of Daunomycin-branched Polypeptide Conjugates" Banoczi Z, Remenyi J, Takeuchi T, Futaki S, Fudeczl F, 42th Japanese Peptide Symposium, Suita, 28 October.

"Peptide Vectors for Intracellular Delivery" Futaki S, 2nd Annual Symposium Japanese-German Frontiers of Sciences, Zushi, 4 November.

Grants

Futaki S, Development of Intracellular Targeting Vectors and the Real-time Observation of the Intracellular Delivery, Grant-in-Aid for Scientific Research (B), 1 April 2005 - 31 March 2008.

Futaki S, Functional Design of Cell-targeting Peptides, PRESTO Program, Japan Science and Technology Agency, 1 November 2002 - 31 October 2005.

Imanishi M, Screening and Evaluation of Novel Clock-related Proteins Using Zinc-finger Technology, PRESTO Program, Japan Science and Technology Agency, 1 October 2005 - 31 March 2009.

A pH-sensitive Fusogenic Peptide to Improve the Transfection Efficiency of Cationic Liposomes

One of the most important steps in intracellular gene-delivery using cationic liposomes is the endosomal escape of the plasmid/liposome complexes to cytosol. The addition of a pH-sensitive fusogenic peptide such as GALA (WEAALAEALAEALAEHLAEALAEALEALAA) may accelerate this step to enhance the expression of the desired proteins. Using representative commercially available cationic liposomes (Lipofectin, Lipofectamine, and Lipofectamine 2000), the effects of GALA on the transfection efficiency were studied by luciferase assay and confocal microscopic observations. A concentration-dependent increase in the transfection efficiency was observed, and addition of 0.1 mM GALA to the plasmid/liposome complex significantly increased the transfection efficiency, especially in the case of Lipofectin. While maintaining a high transfection efficiency, reduction in the liposomal dosage was attained by employing GALA. Although the transfection efficiency was higher in the presence of GALA, a lower amount of the plasmid DNA was taken up by the cells. Confocal microscopic observations of the rhodamine-labeled plasmid show little difference in the cellular localization among cells incubated in the presence or absence of GALA, suggesting that a sublte increase in GALA-induced release of the pasmid to the cytosol may yield a considerable difference in the transfection efficiency. Based on these findings, novel concepts and systems for intracellular gene delivery should be established using pH-sensitive fusogenic peptides.

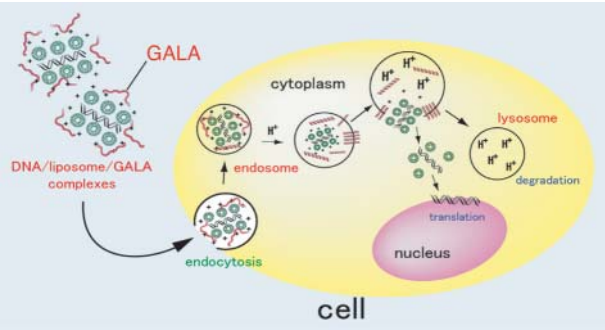


Figure 1. GALA accelerates the endosomal escape of DNA/liposome complexes.

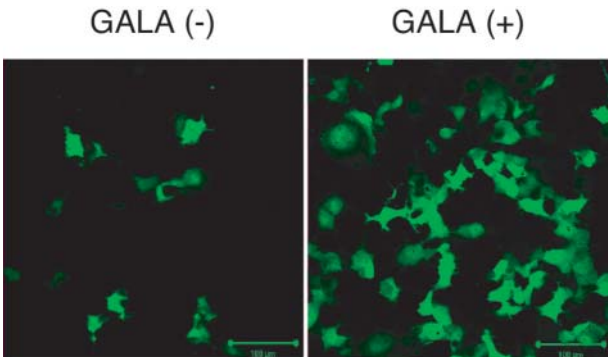


Figure 2. GALA enhances the expression of enhanced green fluorescent protein (EGFP) in COS-7 cells.

Selective Binding to the Discontinuous DNA Sequences by an Artificial Zinc Finger Peptide with Polyarginine Linker

Artificial DNA binding peptides recognizing separated sequences would expand the varieties of the DNA sequences as target sites for transcriptional control. We created a 6-zinc finger peptide, Sp1ZF6(Arg)8, by connecting two DNA binding domains of transcription factor Sp1 with a cationic and bulky polyarginine linker. The DNA binding properties to continuous and discontinuous target sequences were examined and compared to those of Sp1ZF6(Gly)10, which contains a flexible and neutral polyglycine linker. Sp1ZF6(Arg)8 was demonstrated to have an obvious DNA binding preference to discontinuous target sequences, while Sp1ZF6(Gly)10 bound to the both. Footprinting analyses showed that Sp1ZF6(Arg)8 specifically binds to the discontinuous binding sites but not to the continuous ones. Bulky and cationic polyarginine linker may inhibit the suitable binding of Sp1ZF6(Arg)8 to the continuous target sequence, resulting in strong preference to the discontinuous ones. The results provide helpful information for linker design of future zinc finger peptides targeting various states of DNA in addition to desired sequences as gene expression regulators.

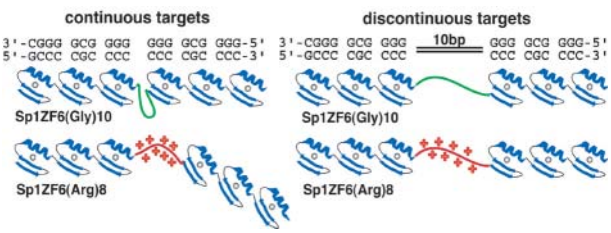


Figure 3. Schematic representation of selective binding of Sp1ZF6(Arg)8 to the discontinuous DNA sequences.

Division of Biochemistry
- Chemistry of Molecular Biocatalysts -

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

Prof
SAKATA, Kanzo
(D Agr)

Assoc Prof
HIRATAKE, Jun
(D Agr)

Assist Prof
MIZUTANI, Masaharu
(D Agr)

Assist Prof
SHIMIZU, Bun-ichi
(D Agr)

PD
CHO, Jeong-Yong
(D Agr)

A Res
SAITO, Shigeki
(D Agr)

A Res
WATANABE, Bunta
(D Agr)

Lecturer (pt)

KATO, Hiroaki (D Agr)
Graduate School of Pharmaceutical Sciences, Kyoto University

Students

KAI, Kousuke (D3)
OHNISHI, Toshiyuki (D3)
HAN, Li-You (D3)
NAKAGAWA, Yuichi (D2)
SAINO, Hiromichi (D2)
AOKI, Nozomu (M2)
FUJIHARA, Fuyuki (M2)
SAKAI, Atsushi (M2)
SAKAI, Eri (M2)
SAKAKI, Yuko (M2)
YASUKAWA, Go (M2)
HASEGAWA, Atsuko (M1)
IDE, Kouhei (M1)
KAMIYAMA, Akane (M1)
TAI, Liz (M1)
TOMOTO, Hiro (M1)
KAWAMURA, Naohiro (RS)

Scope of Research

Our research covers the comprehensive understanding of the physiological roles of biocatalysts (enzymes) as well as the reaction mechanism and specificity of each enzyme. **1)** Studies on diglycosidases specifically hydrolyzing the β-glycosidic bond between disaccharides and aglycons. **2)** Molecular basis of the floral aroma formation in oolong tea. **3)** Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ-glutamyltranspeptidase. **4)** Design and synthesis of novel inhibitors of glycosidases and their application to affinity chromatography and biological probes to understand the physiological roles of glycosidases. **5)** Directed evolutional studies of *Pseudomonas* lipase. **6)** Chemical knockout for probing into IAA homeostasis. **7)** Mechanism of the activation/inactivation process of plant hormones by cytochromes P450. **8)** Molecular mechanism of regulation of phenylpropanoid pathway in plants subjected to various stresses.

Research Activities (Year 2005)

Presentations

Chemical Knockouts for Probing into IAA Homeostasis – Design and Synthesis of Inhibitors of IAA-Amino Acid Conjugate Synthetases, Sakaki Y, Hiratake J, Shimizu B, Mizutani M, Sakata K, 2005 Annual Meeting of Jpn. Soc. Plant Physiologists, Niigata (Niigata), 26 March.

Directed Evolution of Lipase for Improved Amidase Activities – Saturation Mutagenesis of Substrate Binding Site – Hasegawa A, Nakagawa Y, Hiratake J, Sakata K, 2005 Annual Meeting of Kansai Branch of Jpn. Soc. Biosci. Biotech., and Agrochem., Suita (Osaka), 1 October.

Analysis of Coumarin Biosynthesis Pathway in *Arabidopsis thaliana*, Kai K, Shimizu B, Yamaguchi H, Mizutani M, Sakata K, 2005 Annual Meeting of Jpn. Soc. Chemical Regulation of Plants, 1 November.

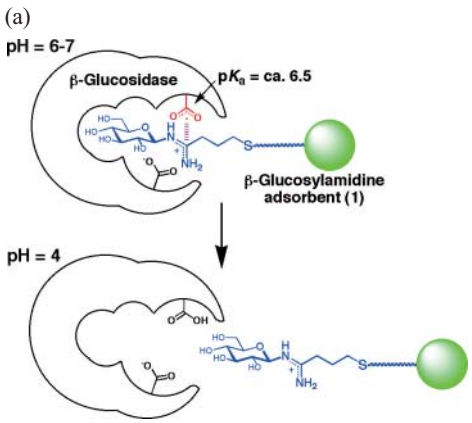
Grants

Sakata K, Studies on Catalytic Mechanism of Disaccharide-specific Glycosidases and Evolution of Plant β-Glucosidases, Grant-in-Aid for Scientific Research (B) (2), 1 April 2004 - 31 March 2007.

Sakata K, Investigation of the Floral Aroma Formation

Controlled Affinity Purification of β-Glucosidases by Using β-Glucosylamidine as Affinity Ligand

β-Glucosylamidines are highly potent and selective inhibitors of β-glucosidases. We found that the inhibitory activity of β-glucosylamidines is attributed largely to the electrostatic interaction between the positively charged amidinium function of the inhibitor and the catalytic acid/base (Glu residue) in the enzyme active site. Hence the affinity of β-glucosylamidines can be controlled by changing the pH of the medium: β-glucosylamidines bind tightly at higher pH where the carboxy residue is deprotonated, while lower affinity results when pH is lowered below the pK_a of the carboxy group (Fig. 1a). This rationale was successfully used for the affinity purification of β-glucosidases from tea leaves. Two enzymes, β-glucosidase 1 and 2, were purified by adsorption to the affinity adsorbent (**1**) at pH 6, followed by elution at pH 4. Each enzyme was eluted sharply immediately after the pH was lowered to give the pure enzymes. The affinity of the β-glucosylamidine (ligand) towards each enzyme was highly dependent on pH: the K_i values were 0.083 and 1.9 μM (for β-glucosidase 1) and 0.017 and 0.62 μM (β-glucosidase 2) at pH 6 and 4, respectively. The controlled affinity purification is applicable widely to various β-glycosidases and may serve as extremely useful chemical tools to study glycosidases.



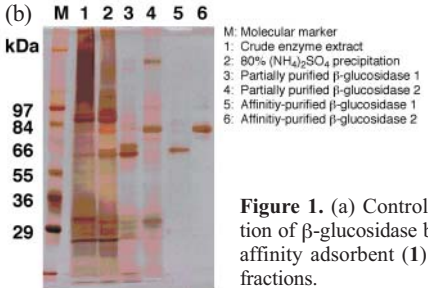


Figure 1. (a) Controlled affinity purification of β-glucosidase by β-glucosylamidine affinity adsorbent (**1**). (b) SDS-PAGE of fractions.

Characterization of P450s Involved in Steroid Hormone Biosynthesis in Plants

Brassinosteroids (BRs) are a group of plant steroids that regulate plant growth and development. Structural variation of BRs comes from the presence of several oxygen moieties at positions C-2, C-3, and C-6 in the A/B-rings and at positions C-22 and C-23 in the side chain. These oxygens are introduced into steroids by several cytochrome P450 monooxygenases (P450s). Arabidopsis *dwf4* is a brassinosteroid (BR) deficient mutant, and the *DWF4* gene encodes a P450, CYP90B1. CYP90B1 activity was measured in an *in vitro* assay, confirming that CYP90B1 is steroid C-22 hydroxylase. The substrate specificity of CYP90B1 indicated that sterols with a double bond at position C-5 are more preferred substrates than stanols, which have no double bond at the position. The results suggest that the C-22 hydroxylation of campesterol before C-5α reduction is the main route, which contrasts with the generally accepted route via campestanol. In addition, CYP90B1 showed C-22 hydroxylation activity toward various $C_{27\text{-}29}$ sterols.

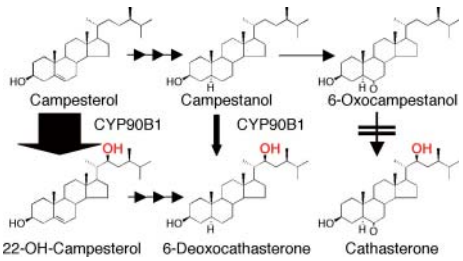


Figure 2. The main routes of the C-22 hydroxylation steps in BR biosynthesis.

Elicited by Leaf-hopper Feeding in Formosa Oolong Tea, Grant-in-Aid for Scientific Research (B) (2), 1 April 2003 - 31 March 2005.

Sakata K, Studies on Glycosidases Hydrolyzing 6-*O*-Modified β-Glucosides by Using Pseudo-sugars as Substrates, Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2005.

Hiratake J, Bio- and Organic Chemical Studies on Plant Glycosidases by Using β-Glycosylamidine Derivatives as Tools, Grant-in-Aid for Scientific Research (B) (2), 1 April 2004 - 31 March 2007.

Hiratake J, Chemical Tools for Probing into IAA Homeostasis – Design and Synthesis of Inhibitors of IAA-Amino Acid Conjugate Hydrolases and Synthetases, Grant-in-Aid for Exploratory Research, 1 April 2005 - 31 March 2006.

Mizutani M, Molecular Mechanisms of the Activation/Inactivation of a Plant Hormone, Grant-in-Aid for Young Scientist B, 1 April 2003 - 31 March 2005.

Division of Biochemistry
- Molecular Biology -

http://molbio.dyndns.org/

Prof
OKA, Atsuhiro
(D Sc)

Assoc Prof
SUGISAKI, Hiroyuki
(D Sc)

Assoc Prof
AOYAMA, Takashi
(D Sc)

Assist Prof
TSUGE, Tomohiko
(D Sc)

Techn
YASUDA, Keiko

Guest Scholar
SERINO, Giovanna
(Ph D)

Guest Res Assoc
LAPARRA, Hélène
(Ph D)

PD
KUSANO, Hiroaki
(D Eng)

Technician (pt)

NAKAGAWA, Shuko

Students

TANIGUCHI, Masatoshi (D3)
IMAI, Kumiko (D3)
TANIGUCHI, Yukimi (D2)
AKI, Shiori (M1)

Visitors

Dr LAPARRA, Hélène	Meristem Therapeutics, France, 1 - 8 April 2005
Prof YOSHIOKA, Keiko	University of Toronto, Canada, 19 May 2005
Assoc Prof SERINO, Giovanna	University of Rome La Sapienza, Italy, 18 August-3 September 2005

Scope of Research

This laboratory aims at clarifying the framework of regulatory network between genetic programs and environmental stress responses through the study on structure-function relationships of genetic materials and cellular proteins in higher plants and pathogens. The current major subjects are the two-component response regulators involved in cytokinin signaling, HD-Zip proteins required for phospholipid signaling, COP9 signalosome modulating protein degradation, and cyclines and CDKs controlling cell cycle.

Research Activities (Year 2005)

Presentations

Transcription Factor-type Response Regulator ARR1 of *Arabidopsis thaliana*: Functions and Target genes, Taniguchi M, Aoyama T, Oka A, International Symposium on Plant Axis Formation and Signal Transduction, 2 - 3 March (Tokyo).

Screening for Genes Directly Regulated by ARR1, Taniguchi M, Aoyama T, Oka A; Novel Regulation of COP9 Signalosome (CSN): a Master Regulator of Signal Transduction in Plant Morphogeneis, Tsuge T, Dohmae N, Wei N, Oka A, 2005 Ann Meeting of Jpn Soc Plant Physiol, 24 - 26 March (Niigata).

Two-component Regulatory System and Cytokinin Signaling, Oka A; COP9 Signalosome: the Key Complex Linking Environmental Signals to Morphogenesis in Plants and Mammals, Tsuge T, Memorial Seminar for the 80th Anniversary of the College of Life Science, Peking University, 29 April (Beijing, PRC).

Screening for the Direct Target Genes of ARR1, Taniguchi M, Aoyama T, Oka A; Revealing the Novel Regulation of COP9 Signalosome (CSN), Tsuge T, Dohmae N, Wei N, Oka A; Expression and Function Analyses of the *AtPLD*ζ2 Gene, Yamamoto Y, Ohashi Y, Oka A, Aoyama, T; AtCYCA2;3 is a Key Regulator in the Termination of Endoreduplication Rounds in *Arabidopsis*, Imai K, Ohashi Y, Tsuge T, Yoshizumi T, Matsui M, Oka A, Aoyama T, XVI International Conference on Arabidopsis Research, 15 - 19 June (Madison, USA).

AtCYCA2;3 is a Key Regulator in the Termination of Endoreduplication Rounds in *Arabidopsis*, Imai K, Ohashi Y, Tsuge T, Yoshizumi T, Matsui M, Oka A, Aoyama T, Rice-Arabidopsis Joint Workshop, 6 - 7 July (Nara).

To Reveal New Mechanisms of CSN: the Key Complex Linking Environmental Signals to Morphogenesis, Tsuge T,

Suppression of CRE1 Defects by Functional Alterations of the Downstream Components

Cytokinins are a class of phytohormones that induce a variety of physiological and developmental events, including cell division. These responses to cytokinins in *Arabidopsis thaliana* (Fig. 1) are triggered through the perception of cytokinin by the sensor histidine kinase CRE1. A *cre1* mutation leads to defect of vascular development, the degree of which depends on each mutant allele. Among those, the *wol* allele show severe inhibition of root growth accompanied by missing phloem, and by frequent generation of short adventitious roots in which the reduced numbers of vascular cells are included [1].

Figure 1. *Arabidopsis* cultivars.

The transcription-factor type response regulators such as ARR1 are activated by cytokinin. On the analogy of bacterial histidine kinases, these response regulators together with the AHP bridge components have been thought to be functionally located downstream of CRE1. CRE1 and ARR1 do not seem to interact directly in cells because of their respective localizations (CRE1 at the cell membrane and ARR1 in nuclei), whereas AHPs seem to be small enough for passive transport through the nuclear membrane (Fig. 2). Indeed, AHP has potential for associating with both CRE1 and ARR1 *in vitro*.

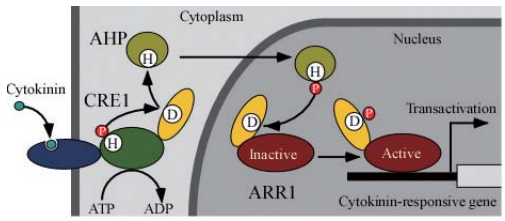


Figure 2. Framework of the intracellular cytokinin signal transduction pathway in *Arabidopsis*. Quoted and altered from ref 1.

From these observations, cytokinin signaling by phosphorelay appears to occur from CRE1 to AHP and then to ARR1 *in vivo* [1]. In order to show that this signal flow actually occurs in plant cells, an attempt was made to suppress *cre1* defects by alterations of the putative downstream components, ARR1 and AHP. Upon introduction into *wol* plants of either constitutively active ARR1ΔR or conditionally active ARR1ΔR::GR, the *wol* phenotype (inhibition of root growth and defect of vascular development) was restored partially to up to a level comparable to that of wild-type plants. These results indicate *cre1* defects being restored by activation of ARR1 without cytokinin, implying that ARR1 is functionally located downstream of CRE1 *in planta*. Another line of suppression mutants were obtained by mutagenesis with *wol* seeds. In addition to several intragenic suppressor mutations, a recessive, extragenic suppressor mutation (*ahp6*) was identified. AHP6 is a pseudo-AHP, and has been presumed to inhibit active AHPs competitively. This suppression also suggests that AHPs work downstream from CRE1. These results support the view that cytokinin signaling in plant cells actually occurs *via* CRE1-AHP-ARR1 phosphorelay, as supposed from a previous biochemical study and from the analogy of bacterial signaling.

[1] Aoyama T & Oka A, *J. Plant Res.*, **116**, 221-231 (2003).
[2] Mähönen A *et al*., *Science*, **311**, 94-98 (2006).

RIKEN Seminar, 10 March (Wako)/ COE Seminar of Nara Institute of Science and Technology, 30 August (Ikoma)/ Institute Seminar of Rome University La Sapienza, 9 September (Rome, Italy).

Characterization of an *Arabidopsis* PI4P5K3 Gene, a Candidate Regulator for Root-hair Development, Kusano H, Yasuda K, Aki S, Ohashi Y, Shimada H, Oka A, and Aoyama T, 1st International Conference on Plant Lipid-Mediated Signaling: Building Connections, 26 - 29 October (Raleigh, USA).

Phospholipid Signaling in Root-hair Cell Morphogenesis, Aoyama T, The 21st Symposium in Conjunction with Award of International Prize for Biology: Morphology, Molecules and Morphogenesis (Awardee: Prof Nam-Hai Chua, Rockefeller Univ), 30 November-1 December (Nagoya).

Novel Regulation of COP9 Signalosome: a Master Regulator of Signal Transduction in Morphogenesis, Tsuge T, Aki S, Dohmae N, Menon S, Wei N, Oka; Functional Analysis of the *AtPIPK3* Gene in Root Hair Development, Kusano H, Yasuda K, Aki S, Yoshizumi T, Matsui M, Oka A, Aoyama T, 2005 Ann Meeting of Mol Biol Soc Jpn, 7 - 10 December (Fukuoka).

Grants

Oka A, Two-component Regulatory System of Phosphorelay Involved in Cytokinin Signaling, Grant-in-Aid for Scientific Research (B), 1 April 2004 - 31 March 2007.

Aoyama T, Roles of Phospholipid Signaling in Root-hair Formation, Grant-in-Aid for Scientific Research (B), 1 April 200 - 31 March 2007.

Division of Biochemistry
- Chemical Biology -

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

Prof
UESUGI, Motonari
(D Pharm Sc)

Assoc Prof
TANAKA, Seigo
(D Med Sc)

Assist Prof
KAWAZOE, Yoshinori
(D Med Sc)

PD
SATO, Ayato
(D Sc)

Researcher

Prof Em UEDA, Kunihiro (D Med Sc)

Students

TAKAGI, Junpei (D2)
KONDO, Eriko (M1)
NAKAJIMA, Risa (M1)
KITAJIMA, Takashi (RS)

Visitors

Prof SAZER, Shelley	Baylor College of Medicine, USA, 28 September 2005
Prof HAN, Kyou Hoon	Korea Research Institute of Bioscience and Biotechnology, Korea, 8 November 2005
Prof SUZUKI, Hisanori	University of Verona, Italy, 30 November 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, 78th National Meeting of Japanese Society of Pharmacology, Yokohama, Japan, 22 - 24 March 2005.

Modulation of Gene Expression by Targeting a Protein-protein Interaction, Uesugi M, 12th International Molecular Medicine Tri-Conference, San Francisco, USA, 19 - 22 April 2005.

Synthetic Small Molecules that Modulate Gene Expression and Cell Differentiation, Uesugi M, 20th International Combinatorial Chemistry Symposium, Osaka, Japan, 25 - 26 April 2005.

Poly(ADP-ribose)polymerase-1 Activation and Mitochondrial Impairment *in vitro* Model of Cerebral Ischemia, Tanaka S, 20th Biennial Meeting of the ISN Satellite Symposium "Molecular Basis for Signal Transduction in Neurodegeneration and Neuroregeneration", Warsaw, Poland, 26 August - 1 September 2005.

Poly(ADP-ribose)polymerase-1 Activation and Mitochondrial Impairment in *in vitro* Model of Cerebral ischemia, Tanaka S, 18th National Convention on ADP-ribosylation Process, Verona, Italy, 3 - 4 October 2005.

Regulation of NF-κB and AP-1 by PARP-1 in Reactive Astrocytes of Alzheimer's Disease, Tanaka S, 14th International Meeting of ADP Ribosylation Reactions, "PARP2005: Bench to Bedside", Newcastle, UK, 5 - 7 October 2005.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, 6th Australian Peptide Conference, Hamilton Island, Queensland, Australia, 9 - 14 October 2005.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, Pacifichem 2005 Symposium, "Chemical Biology: Small Chemical Compounds As Magic Bullets To Elucidate Biological Mechanisms", Honolulu, Hawaii, 15 - 20 December 2005.

Grants

Uesugi M, Small Molecule Transcription Factors that

Small-Molecule-initiated Biology

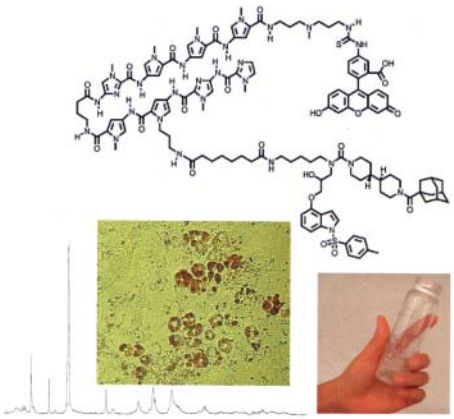
Our current research programs focus on discovering and designing small organic molecules that modulate gene transcription or cell differentiation and using them as tools to explore biology. Regulation of gene transcription and cell differentiation often induces drastic phenotypic changes in living organisms.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

Discovery of organic compounds that modulate transcription. Our group isolated human Sur-2, a Ras-linked subunit of the human mediator complex, as a nuclear factor that plays a critical role in overexpression of Her2 in breast cancer cells. This achievement was well appreciated in the oncology field because Her2 is a clinically important oncogene whose overexpression occurs in ~30% of breast cancer patients. Our group showed, by a combination of biochemical and NMR experiments, that Sur-2 protein interacts with a short alpha-helical motif in the activation domain of ESX transcription factor to activate Her2 transcription.

We also discovered a small-molecule inhibitor of the ESX-Sur2 interaction by a screening of a focused chemical library. The compound that we named "adamanolol" represents the first small molecules that modulate gene transcription by targeting transcription factor-coactivator interaction. Our group, as a collaboration with another laboratory, synthesized adamanolol and its derivatives and obtained structure-activity relationship, which enabled the design of the second-generation compound named "wrenchnolol." The wrench-shaped compound is now recognized in the field as a highly unique synthetic molecule that controls gene expression.

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

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



Roles of Poly(ADP-ribose) polymerase-1 in Alzheimer's Disease

Poly(ADP-ribose) polymerase-1 (PARP-1) is a nuclear enzyme that catalyzes formation of $(ADP\text{-}ribose)_n$ chains on acceptor proteins including histones and PARP-1 itself. PARP-1 is termed a "guardian of the genome", because it assists DNA repair by sensing DNA damage. In the present year, our group investigated a role of PARP-1 in transcriptional regulation and Alzheimer's disease (AD) pathogenesis. Our group examined the effects of PARP-1 siRNA on the DNA-binding activities of a range of transcription factors. Among transcription factors examined, NF-κB and AP-1 were found to increase their DNA binding activity in astrocytes after the addition of β-amyloid, whereas the increase of their DNA-binding was suppressed by PARP-1 siRNA in a dose-dependent manner. NF-κB and AP-1 are the transcription factors involved primarily in expression of proinflammatory or cytotoxic factors in AD astrocytes, and PARP-1 plays a critical role as a coactivator in their transcriptional activation. It is an exciting prospect that manipulation of the PARP-1 expression may serve as a novel therapeutic intervention in the treatment of AD.

can be Used for Biological Investigation, Precursory Research for Embryonic Science and Technology, Japan Science and Technology Agency, 1 October 2005 - 31 March 2009.

Tanaka S, Study on the Function of NAD^+ and ADP-ribose as Stress Mediator, Japan Foundation for Applied Enzymology, 1 April 2005 - 31 March 2006.

Division of Environmental Chemistry
- Molecular Materials Chemistry -

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

Prof
HORII, Fumitaka
(D Eng)

Assoc Prof
KAJI, Hironori
(D Eng)

Assist Prof
HIRAI, Asako
(D Eng)

Techn
OHMINE, Kyoko

A Res
LUO, Qing
(D Sc)

PD
YANG, Hu
(D Sc)

PD
JIA, Yinggang
(D Eng)

Students

SUZUKI, Furitsu (M2)
YAMADA, Tomonori (M2)
SHIMADA, Junya (M2)
KANIE, Yasumasa (M1)
MINO, Akira (M1)
INUI, Osamu (UG)
SESEI, Takashi (UG)

Visitors

Prof MARCHESSAULT, Robert H — R H, Xerox Research Centre of Canada, Canada, 26 - 27 October 2005
Dr SAMOSON, Ago — National Institute for Chemical Research and Biophysics, Estonia, 12 - 14 November 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Possible Origin of Disordered Structure in Bacterial Cellulose: Structure and Structural Evolution of Sub-Elementary Fibrils, Horii F, 229th ACS National Meeting, San Diego, March 13 - 15 (Invited).

Solid-State NMR Analyses of the Structure and Dynamics of Hydrogen-Bonded Polymers, Horii F, POLYCHAR-14 (Symposium U of ICMAT and ISPAT), Singapore, July 3 - 8 (invited).

Noncrystalline Structure of Native and Synthetic Polymer Materials, Horii F, Soc. Fiber Sci. Technol., June 8 - 10 (Invited).

Super-High Field Solid-State NMR Characterization of Polymer Materials, Horii F, PACIFICHEM 2005, 15 - 20 December (Invited).

The Disordered Structure of Native Cellulose and the Origin of the Formation, Horii F, PACIFICHEM 2005, 15-20 December (Invited).

Solid-State NMR Investigations of Materials in Organic Light-Emitting Diodes, Kaji H, PACIFICHEM 2005, 15 - 20 December (Invited).

Isomeric States and Molecular Packing in Alq_3 Polymorphs Studied by CP/MAS ^{13}C NMR, Kaji H, Third International Conference on Molecular Electronics and Bioelectronics (M&BE3), 3 - 4 March.

Conformational Analysis of TPD by Two-Dimensional Solid-State Double-Quantum NMR Spectroscopy and Quantum Chemical Calculations, Yamada T, Tsukamoto N, Kaji H, and Horii F, The 44th Annual Meeting of Japanese NMR Society and The 1st Asia-Pacific NMR Symposium, November 10, 2005.

Phase Behavior of Aqueous Mixtures of Cellulose Microfibrils and Imogolite Nanotubes and Preparation of Their Nanocomposites, Hirai A, PACIFICHEM 2005, 15 -

Relationships between Light-Emitting Properties and Isomeric States in Alq_3 Polymorphs Studied by Solid-State ^{27}Al NMR[1]

Tris-(8-hydroquinoline) aluminum (Alq_3) is one of the most widely used light-emitting and electron-transport materials in organic light emitting diodes (OLEDs). Recently, Brinkmann et al. found three crystalline forms, α-, β-, and γ-Alq_3, and the crystalline structures of α- and β-Alq_3, both are composed of only the meridional isomer, were determined. In contrast, the crystalline structure of γ-Alq_3 has been still unclear. More recently, Braun et al. found a new crystalline phase, δ-Alq_3. This shows interesting features; blue luminescence and a high photoluminescence quantum yield (51 %). Alq_3 is normally in the amorphous state in organic EL devices and the analysis of the amorphous structure is also crucial. In this study, isomeric states of Alq_3 in the different polymorphs, α-, γ-, δ-Alq_3, and in the amorphous state have been analyzed by solid-state NMR measurements.

Figure 1 shows the experimental ^{27}Al magic angle spinning (MAS) NMR spectra of Alq_3 in the different states. MAS technique eliminates the effect of chemical shift anisotropy and the spectra only reflect the quadrupolar interaction. Therefore, information on electric field gradient (EFG) tensors is obtained. For α-Alq_3 and amorphous Alq_3, broad spectral patterns are observed, whereas γ-Alq_3 and δ-Alq_3 give sharp spectral patterns. Qualitatively, these results show that the EFG tensors are more axially symmetric for γ- and δ-Alq_3 compared to α- and amorphous Alq_3. The quantitative symmetry is obtained by the asymmetry parameters, η. Although the spectra of α- and amorphous Alq_3 are not well reproduced by simulations up to now, the values of η are considered to be 0.6 – 1.0, which suggest Alq_3 molecules in these samples are in the meridional form. The simulations for γ- and δ-Alq_3 well reproduce the experimental spectra, and from the best-fit simulations, the values of η are determined to be 0 and 0.24, respectively. The DFT calculation for a single facial Alq_3 molecule predicts the axially symmetric pattern with $\eta = 0$. The DFT calculated value is in excellent agreement with the experimentally determined value for γ-Alq_3 ($\eta = 0$) and we conclude that the γ-Alq_3 is composed of the facial isomer. The point charge model calculation for facial Alq_3 in the δ-crystalline form gives $\eta = 0.26$. This value agrees well with our ^{27}Al MAS NMR result, $\eta = 0.24$, indicating the non-zero η value for δ-Alq_3 is originated from the crystalline intermolecular packing. We can therefore conclude that α- and amorphous Alq_3 are composed of the meridional isomer, whereas γ- and δ-Alq_3 are composed of the facial isomer.

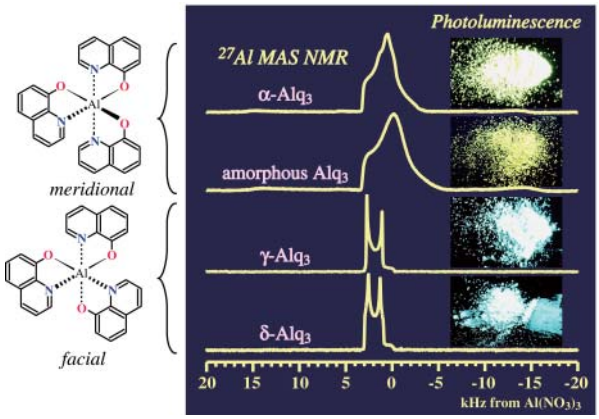


Figure 1. MAS ^{27}Al NMR spectra of α-, amorphous, γ-, and δ- Alq_3.

Our α- and amorphous Alq_3 samples show fluorescence spectra with maxima at 510 and 509 nm, respectively. In contrast, blue-shifted fluorescences are observed for γ- and δ-Alq_3 whose maxima are at 468 and 466 nm, respectively. This clearly indicates a close relation between the isomeric states and the light-emitting properties.

[1] H. Kaji, Y. Kusaka, G. Onoyama, F. Horii, Jpn. J. Appl. Phys., 2005, 44, 3706.

20 December (Invited).

Liquid Crystal Structure of Nanocomposites of Cellulose Microfibrils and Imogolite Nanotubes, Ikuno M, Hirai A, Horii F, Donkai N, Tsuji M, 54th Annual Meeting, Soc. Polym. Sci., Jpn., 25 May.

Grants

Horii F, Precise Solid-State NMR Analyses of Non-crystalline Organized Structure and Dynamics of Polymer Functional Materials, Grand-in-Aid for Scientific Research (B)(2), 1 April 2004 - 31 March 2006.

Horii F, Hybridization Utilizing Hierarchical Structure of Microbial Cellulose by a Newly Developed Microbio-system, Grand-in-Aid for Scientific Research, 1 April 2004 - 31 March 2006.

Kaji H, Higher Order Structures and Optical Properties of Light-Emitting Polymeric Materials, PRESTO, Japan Science and Technology Agency, 1 November 2002 - 31 March 2006.

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

Kaji H, Development of Sublimation NMR Method, Grant-in-Aid for Scientific Research, 1 April 2005 - 31 March 2007.

Division of Environmental Chemistry
- Hydrospheric Environment Analytical Chemistry -

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

Prof
SOHRIN, Yoshiki
(D Sc)

Assoc Prof
UMETANI, Shigeo
(D Sc)

Assist Prof
SASAKI, Yoshihiro
(D Sc)

Assist Prof
OKAMURA, Kei
(D Sc)

Res Associate
NORISUYE, Kazuhiro
(D Sc)

Techn
MINAMI, Tomoharu

Students

KINUGASA, Masatoshi (D3)
KURAHASHI, Kensuke (D3)
MOCHAMAD, Lutfi Firdaus (D2)
NAKATSUKA, Seiji (D1)
MATSUNARI, Takahiro (M2)
SATO, Taishi (M2)
TAGUCHI, Yusuke (M2)
NAKAGAWA, Yusuke (M1)
TERUI, Daisuke (M1)
URUSHIHARA, Shohei (M1)

Scope of Research

Research activities are concerned with geochemistry, oceanography, limnology and analytical chemistry, which are important basic sciences in order to realize the sustainable society. Major research subjects are as follows: (i) Biogeochemistry of trace elements in the hydrosphere. (ii) Hydrothermal activity and deep biosphere on the ocean floor. (iii) Fe-uptake mechanism of phytoplankton. (iv) Ion recognition. (v) Simulation of non-linear chemical reaction.

Research Activities (Year 2005)

Presentations

Determination of Chromium, Copper and Lead in River Water by Graphite-Furnace Atomic Absorption Spectrometry after Coprecipitation with Terbium Hydroxide, Minami T, Sohrin Y, Ueda J, The 54th Annual Meeting of the Japan Society for Analytical Chemistry, 15 September 2005.

Determination of Dissolved Zr, Hf, Nb, Ta and W in the North Pacific Ocean, Firdaus M L, Norisuye K, Sohrin Y, The 52nd Annual Meeting of the Geochemical Society of Japan, 26 September 2005.

Trace Metals and Biological Processes in the Ocean, Norisuye K, Sohrin Y, The 2005 Fall Meeting of the Oceanographic Society of Japan, 1 October 2005.

Geochemistry of Bioactive Trace Metals during an *In-situ* Iron Enrichment in the Subarctic Western North Pacific Gyre (SEEDS II), Nakatsuka S, Nishioka J, Kinugasa M, Sohrin Y, SEEDS II Workshop Second Iron Enrichment Experiment in the Western Subarctic Pacific, 17 October 2005.

Hydrothermal Plumes at the Myojinsho Submarine Caldera, the Shicitio-Iwojima Ridge, Izu-Bonin Arc, Okamura K, Toki T, Hyun K S, American Geophysical Union Fall Meeting 2005, 9 December 2005.

Selective Separation of Zn(II) and Cd(II) Using Nitrogen Containing Macrocyclic Ligands as Ion-Size Selective Masking Reagents, Kurahashi K, Taguchi Y, Umetani S, Sohrin Y, Pacifichem 2005, 17 December 2005.

Molecularly Imprinted Sol-Gel Materials for the Separation of Metal Ions, Taguchi Y, Kurahashi K, Umetani S, Sohrin Y, Pacifichem 2005, 17 December 2005.

Grants

Sohrin Y, Interaction between Metallome and Proteome in the Marine Ecosystem, Grant-in-Aid for Scientific Research (A) (2), 1 April 2004 - 31 March 2007.

Okamura K, Development of Time-series Measurement System of Sulfur Related Matter in Seawater, Grant-in-Aid for Young Scientists B, 1 April 2003 - 31 March 2006.

Okamura K, Transportation of Trace Heavy Metal to Natural Water from Exhaust Gas, Nissan Science Foundation, 1 April 2005 - 31 March 2006.

Geochemistry of Bioactive Trace Metals during the Mesoscale Iron Enrichment in the Subarctic Western North Pacific Gyre (SEEDS I and II)

The equatorial Pacific, the North Pacific and the Southern Ocean are well known as high-nutrient low-chlorophyll (HNLC) regions, where phytoplankton biomass is low (<1 μg Chl *a* l^{-1}) despite abundance of macronutrients (NO_3^-, PO_4^{3-}, $Si(OH)_4$). In most HNLC waters, low concentration of dissolved iron (<0.22 μm) was identified, using extremely careful sampling and analytical techniques. Iron has been invoked as a limiting factor to primary production (iron hypothesis) due to its biological requirement, together with light-limitation, grazing effect by zooplankton and water temperature. Recently, the iron hypothesis is evidenced by the fact that a number of mesoscale iron enrichment resulted in a rapid accumulation of phytoplankton biomass. We have been investigated the marine geochemistry of Fe, Co, Ni, Cu, Zn and Cd, which have many implications for phytoplankton's growth and metabolic processes, during the mesoscale iron enrichment in the Subarctic Western North Pacific Gyre (SEEDS I and II: in the cruise of Hakuho-Maru, Fig. 1).

Figure 1. Hakuho-Maru; the research vessel used for the observation during SEEDS I and II.

SEEDS I and II have been conducted in 2001 and 2004, respectively. Although both experiments showed increase in primary production, the effect was very different: SEEDS I resulted in a massive increase in biomass (20 μg/kg of Chl *a*) with floristic shift to fast-growing centric diatom *Chaetoceros debilis*, whereas the response in SEEDS II was much less significant (~3 μg/kg of Chl *a*) with domination of Pennate diatom *Pseudo Nitzschia*. High density of mesozooplankton biomass (*copepod*) was also observed in SEEDS II. During SEEDS II, bottle incubation was conducted using ambient seawater, from which mesozooplankton was removed. The bottle incubation revealed that addition of iron (1 nM) triggered increase in Chl *a* up to ~9 μg/kg, shown in Fig. 2.

In SEEDS I (for 13 days), the concentration of dissolved Co, Ni, Cu, Zn and Cd decreased by 0.03, 0.7, 0.4, 1.3 and 0.06 nM, respectively, following development of the bloom. It was the first observation that Co, Ni, Cu and Zn decreased by the iron enrichment. Compared to SEEDS I, SEEDS II (for 32 days) exhibited a quite different response. There was no major decrease in the concentration of trace metals except for Cd (~0.2 nM). In contrast, the concentration of trace metals during the bottle incubation showed significant decreases in dissolved Zn (~0.3 nM) and Cd (~0.2 nM). The variations of trace metals are shown in Fig. 3.

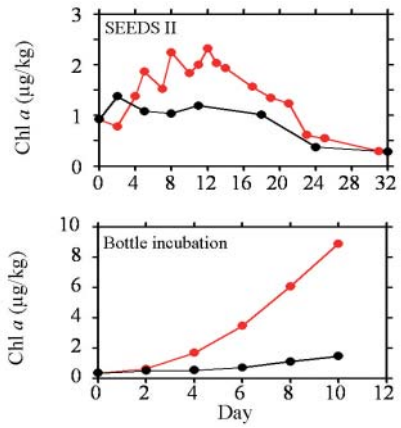


Figure 2. The increase in Chl *a* during SEEDS II and bottle incubation. The red symbol with solid line and the black one indicate the iron enriched and ambient seawater, respectively.

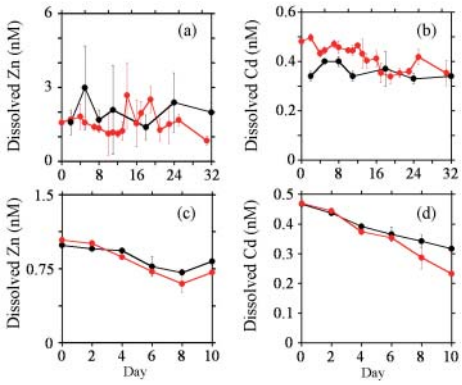


Figure 3. The variation of the trace metals in surface mixed layer during SEEDS II (a and b) and the bottle incubation (c and d). The red symbol with solid line and black one indicate the iron-enriched sea water and the bottles received iron, respectively.

On the basis of the iron enrichment and the bottle incubation, it can be concluded that phytoplankton plays a primary roll in controlling the concentration of trace metals through active uptake in the ocean. Zooplankton also appears to be controlling the concentration of trace metals indirectly, through the grazing effect on phytoplankton.

Division of Environmental Chemistry
- Solution and Interface Chemistry -

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

Prof
NAKAHARA, Masaru
(D Sc)

Assoc Prof
MATUBAYASI, Nobuyuki
(Ph D)

Assist Prof
OKAMURA, Emiko
(D Pharm Sc)

Assist Prof
WAKAI, Chihiro
(D Sc)

PD
KIMURA, Tomohiro
(D Sc)

Students

MIKAWA, Kohei (D2)
GIORDANI, Cristiano (D2)
MOROOKA, Saiko (D1)
YOSHIDA, Ken (D1)
KINOSHITA, Tomoko (M1)
KURITA, Naoyoshi (M1)
YASAKA, Yoshiro (M1)

Visitors

Dr CHAU, Pak-Lee	Bioinformatique Structurale Institut Pasteur, France, 12 January 2005
Prof TANG, Pei	University of Pittsburgh School of Medicine, USA, 28 February 2005
Prof KLEIN, Michael L.	University of Pennsylvania, USA, 14 April 2005
Prof MARONCELLI, Mark	The Pennsylvania State University, USA, 11 October 2005
Prof SAVAGE, Phillip E.	University of Michigan, USA, 7 - 19 November 2005

Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR and computer simulations from ambient to extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Static and dynamic NMR of endocrine disruptors, anesthetics, peptides, and proteins in model and cell membranes are also investigated.

Research Activities (Year 2005)

Presentations

Mobility and Location of Anesthetics in Lipid Bilayer Membranes by High-Resolution, High-Field-Gradient NMR, Okamura E, Nakahara M, The 7th International Conference on Mechanisms of Anesthesia, 25 - 27 February.

Molecular Dynamics Simulation of Solubilization by Micelle, Liang Kuo-Kan, Matubayasi N, Nakahara M, The 85th Annual Meeting of the Chemical Society of Japan, 26 - 29 March, and 3 related presentations in other symposia.

Limited Slowdown of Molecular Diffusion in Confined Fluid Lipid Membranes, Okamura E, Wakai C, Matubayasi N, Nakahara M, The 72nd Meeting of the Electrochemical Society of Japan, 1 - 3 April (Invited), and 6 related presentations in other meetings and symposia.

Method of Energy Representation as an Approach to the Solvation Free Energy, Matubayasi N, EMLG/JMLG Annual Meeting 2005 (Invited), 4 - 8 September, and 5 related presentations in other meeting, symposium, and conference.

Self-Diffusion of Light and Heavy Water in Sub- and Supercritical Conditions Studied by a New High-Temperature Multinuclear Diffusion NMR Probe, Yoshida K, Wakai C, Matubayasi N, Nakahara M, The General Symposium of Molecular Structure, 27 - 30 September, and 3 related presentations in other meetings and symposium.

Multinuclear NMR Study on Rotational Dynamics for Imidazolium-based Ionic Liquids, Wakai C, Matubayasi N, Nakahara M, 28th Symposium on Solution Chemistry of Japan, 17 - 19 November.

A New Hydrothermal C1 Chemistry: C-C Bond Formation and Disproportionations of Formaldehyde and Formic Acid, Morooka S, Wakai C, Matubayasi N, Nakahara M, Pacifichem 2005, 15 - 20 December, and 6 related presentations in other meetings and symposia.

Grants

Nakahara M, Development of Multinuclear, High-Temperature, and Diffusion Measurable NMR Probe and

A New High-Temperature Multinuclear-Magnetic-Resonance Probe and the Self-Diffusion of Light and Heavy Water in Sub- and Supercritical Conditions

A high-resolution nuclear magnetic resonance (NMR) probe (500 MHz for ^{1}H, Figure 1) has been developed for multinuclear pulsed field gradient spin-echo (PGSE) diffusion measurements at high temperatures up to 400 °C. The high precision is achieved by the homogeneous temperature distributions dramatically improved. The self-diffusion coefficients D for light (^1H_2O) and heavy (^2H_2O) water are distinguishably measured at subcritical temperatures of 30-350 °C on the liquid-vapor coexisting curve and at a supercritical temperature of 400 °C as a function of water density between 0.071 and 0.251 g/cm^3. The D value obtained for ^1H_2O is 10-20% smaller than those previously reported because of the absence of the convection effect. At 400 °C, the D value for ^1H_2O is increased by a factor of 3.7 as the water density is reduced from 0.251 to 0.071 g/cm^3. The isotope ratio $D(^1H_2O)/D(^2H_2O)$ decreases from 1.23 to ~1.0 as the temperature increases from 30 to 400 °C.

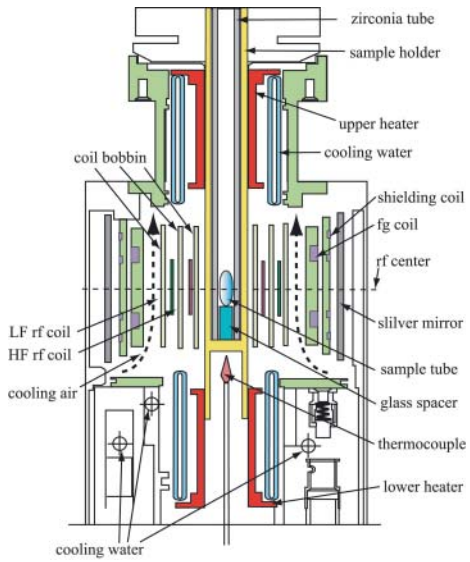


Figure 1. The cross-section view of the high-temperature multinuclear diffusion NMR probe.

Hydrothermal Carbon-Carbon Bond Formation and Disproportionations of C1 Aldehydes: Formaldehyde and Formic Acid

Hydrothermal reaction pathways and kinetics of C1 (carbon-one) aldehydes, formaldehyde (HCHO) and formic acid (HCOOH = HOCHO), are studied at 225 °C without and with hydrochloric acid (HCl) up to 0.6 M (mol dm^{-3}). Reactions unveiled are: (i) the self-disproportionation forming methanol and formic acid, a redox reaction between two formaldehydes, (ii) the cross-disproportionation forming methanol and carbonic acid, a redox reaction between formaldehyde and formic acid, and (iii) the acid-catalyzed C-C bond formation producing glycolic acid ($HOCH_2COOH$) as a precursor of the simplest amino acid, glycine (Figure 2). The reaction (iii) is a hydrothermally induced chemical evolution step from C1 aldehydes, formaldehyde and formic acid. The disproportionations (i) and (ii) are found to proceed even without base catalysts unlike the classical Cannizzaro reaction. The yield of ~90% for the glycolic acid formation and that of ~80% for the methanol formation are experimentally achieved, respectively, as a result of path weight control based on the kinetic analysis.

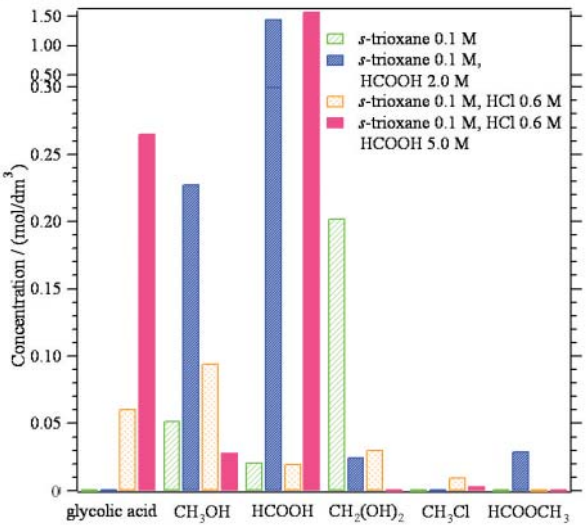


Figure 2. The product concentrations in various reaction conditions. The ordinate scale is changed at 0.30 mol/dm^3.

Molecular Analysis of Dynamics of Supercritical Aqueous Solutions, Grant-in-Aid for Scientific Research (A), 1 April 2003 - 31 March 2006.

Nakahara M, Free-Energy Analysis of Nanoscale Aggregates of Molecules in the Method of Energy Representation, National Research Grid Initiative Project, 1 April 2003 - 31 March 2008.

Matubayasi N, Molecular Theory of the Solvation Effect on the Structural Formation and Fluctuation of Biomolecules and their Aggregates, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2003 - 31 March 2008.

Matubayasi N, Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2004 - 31 March 2006.

Okamura E, Molecular Dynamics in Lipid Rafts by High-Sensitivity, High-Resolution NMR, Grant-in-Aid for Scientific Research (C), 1 April 2005 - 31 March 2007.

Division of Environmental Chemistry
- Molecular Microbial Science -

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

Prof
ESAKI, Nobuyoshi
(D Agr)

Assoc Prof
KURIHARA, Tatsuo
(D Eng)

Assist Prof
MIHARA, Hisaaki
(D Agr)

Res Associate
KAZUOKA, Takayuki
(D Eng)

PD (JSPS)
OMI, Rie
(D Sc)

PD (JSPS)
KATO, Dai-ichiro
(D Sc)

Guest Res Assoc
AI NOI, Sauvaphap

Technicians (pt)

TANAKA, Yumi
UTSUNOMIYA, Machiko
MURAMATSU, Misa

Students

ABE, Katsumasa (D2)
KAWAMOTO, Jun (D2)
MIYAKE, Ryoma (D2)
KUROKAWA, Suguru (D1)
OMORI, Taketo (D1)
YAMAUCHI, Takae (D1)
HATA, Chikako (M2)
INOMOTO, Yasushi (M2)
JITSUMORI, Keiji (M2)
MURAI, Ken (M2)
MURAKAMI, Yoshiko (M2)
OSAKI, Motoharu (M2)
TAGO, Tsukasa (M2)
UEMURA, Tadashi (M2)
NISHIJIMA, Yoshihito (M1)
OMORI, Yukiko (M1)
SHIGAKI, Yuta (M1)
TANAKA, Nobutoshi (M1)
YAMAMOTO, Kentaro (M1)
YOKOYAMA, Izumi (M1)
ZHANG, Wanjiao (M1)
HIDESE, Ryota (RS)

Scope of Research

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

Research Activities (Year 2005)

Presentations

An Enzyme Usuful for the Synthesis of Optically Active *N*-Alkyl Amino Acids and Cyclic Imino Acids, Mihara H, Muramatsu H, Kakutani R, Yasuda M, Ueda M, Kurihara T, Esaki N, The 57th Annual Meeting, Vitamin Soc. Jpn., 27 May.

Iron-sulfur Cluster Assembly by Suf Proteins of *Escherichia coli*, Kazuoka T, Mihara H, Kurihara T, Esaki N, 2005 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 30 March.

Morphological Changes of a Psychrotrophic Bacterium, *Shewanella* sp. Ac10, Depending on Cultivation Temperatures, Kawamoto J, Kurihara T, Kitagawa M, Asada K, Esaki N, 2005 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 30 March.

Mechanism of Selenocysteine Lyase from Rat, Kurokawa S, Mihara H, Kurihara T, Esaki N, 2005 Annual Meeting, Jpn. Biochem. Soc., 20 October.

Detection of Phosphatidylthreonine in Porcine Brain and It's Localization, Omori T, Kazuoka T, Mihara H, Kurihara T, Esaki N, 2005 Annual Meeting, Jpn. Biochem. Soc., 21 October.

Identification of Amino Acid Residues Essential for Hydrolytic Defluorination by Fluoroacetate Dehalogenase, Jitsumori K, Kurihara T, Omi R, Miyahara I, Hirotsu K, Esaki N, 2005 Annual Meeting, Jpn. Biochem. Soc., 20 October.

Grants

Esaki N, Dynamics of an Essential Trace Element, Selenium, in Mammals and the Molecular Basis of Selenoprotein Biosynthesis, Grant-in-Aid for Scientific Research (B),

Structure and Reaction Mechanism of Fluoroacetate Dehalogenase

Fluoroacetate dehalogenase from *Burkholderia* sp. FA1 (FAc-DEX FA1) catalyzes the hydrolytic dehalogenation of haloacetates. Although the carbon-fluorine bond is stronger than other carbon-halogen bonds, the enzyme shows the highest activity toward fluoroacetate. The activities toward chloroacetate and bromoacetate were less than 5% of the activity toward fluoroacetate. In order to elucidate the reaction mechanism of the enzyme, we determined the three-dimensional structures of the native FAc-DEX FA1, the D104A FAc-DEX FA1 complexed with the substrate, and the H271A FAc-DEX FA1 ester-intermediate. We found that Arg105, Arg108, His149, Trp150, and Tyr212 had short contacts with the substrate fluoroacetate. When Trp150, which interacts with the carboxylate group of the substrate, was replaced with Ala, the activity toward fluoroacetate was completely lost: the K_m and V_{max} values of the wild-type enzyme for fluoroacetate were 9.1 mM and 61 μmol/min/mg, respectively, whereas the W150A mutant enzyme showed no activity toward fluoroacetate. In contrast, the activity toward chloroacetate was not significantly affected by the same mutation: the K_m and V_{max} values of the wild-type enzyme were 15 mM and 2.6 μmol/min/mg, respectively, and the K_m and V_{max} values of W150A were 24 mM and 2.0 μmol/min/mg, respectively. Thus Trp150 is specifically required for the defluorination. Structural comparison between the W150A mutant enzyme and the wild-type enzyme would give us a clue for clarifying how the enzyme catalyzes the cleavage of carbon-fluorine bond.

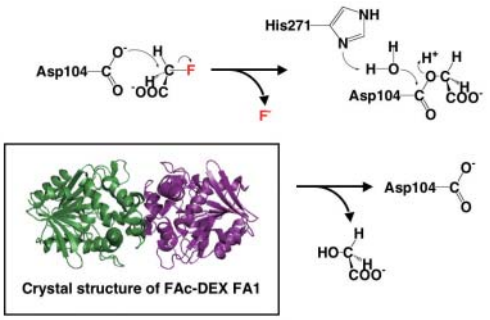


Figure 1. Structure and reaction mechanism of FAc-DEX FA1.

Enzymatic Synthesis of L-pipecolic Acid by Δ^1-piperideine-2-carboxylate Reductase from *Pseudomonas putida*

Optically active L-pipecolic acid occurs as constituents in several biologically active natural products. Therefore optically pure L-pipecolic acid is thought to be useful building blocks of medicines and pesticides. We found Δ^1-piperideine-2-carboxylate (Pip2C) reductase in *Pseudomonas putida*. Pip2C reductase catalyzes the NADPH-dependent synthesis of L-pipecolic acid from Δ^1-piperideine-2-carboxylic acid. Recombinant *E. coli* BL21(DE3) expressing both Pip2C reductase and glucose dehydrogenase was constructed. A crude extract of the cells was obtained by sonication and centrifugation. L-Pipecolic acid was synthesized in a reaction mixture containing 1.5 mg-protein/ml crude extract, 1.5 U/ml L-lysine oxidase, 14 U/ml catalase, 1% L-lysine, 100 mM glucose, 0.2 mM $NADP^+$, 1.0 mM FAD and 100 mM Tris-HCl (pH 7.5) at 30°C and with reciprocal shaking. After 5 hr, 0.5% L-lysine, 50 mM glucose and 7 U/ml catalase were added to the reaction mixture. L-Lysine and L-pipecolic acid were determined by HPLC. After 15-hr reaction, 14 g/l L-pipecolic acid was obtained (98% yield). Optical purity of the product was analyzed by HPLC and determined to be >99% e.e.

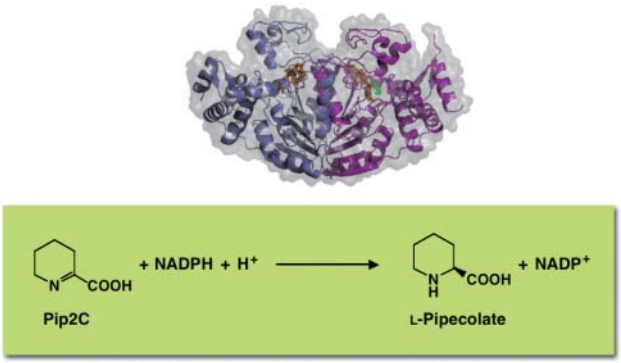


Figure 2. Crystal structure and catalytic reaction of Pip2C reductase.

1 April 2005 - 31 March 2007.

Kurihara T, Conversion of Organofluorine Compounds with Microbial Enzymes: Mechanistic Analysis of the Enzyme Reactions and Their Application to Production of Useful Compounds and Bioremediation of Environments, Grant-in-Aid for Scientific Research (B), 1 April 2005 - 31 March 2007.

Kurihara T, Exploration of Novel Cold-adapted Microorganisms That Inhabit the Polar Regions and Investigation of Their Useful Enzymes, Grant-in-Aid for Scientific Research (B), 1 April 2005 - 31 March 2007.

Mihara H, Mechanisms of Incorporation of Sulfur and Selenium into the Anticodon Wobble Bases of tRNAs, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2006.

Division of Multidisciplinary Chemistry
- Polymer Materials Science -

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

Prof
KANAYA, Toshiji
(D Eng)

Assoc Prof
NISHIDA, Koji
(D Eng)

Assist Prof
MATSUBA, Go
(D Eng)

PD
KAWAI, Takahiko
(D Eng)

Students

KONISHI, Takashi (D3)
OGINO, Yoshiko (D3)
OGAWA, Hiroki (D2)
INOUE, Rintaro (D1)
TAKEDA, Taijiro (M2)
SAKAMOTO, Shinya (M2)
TSUBOUCHI, Tsuyoshi (M2)
TAKAYAMA, Yoshiyuki (M2)
AKAI, Wataru (M1)
ISEKI, Toru (M1)
HIRABAYASHI, Tetsuo (M1)
TAKAHASHI, Naoya (B4)
YAMAMOTO, Junpei (B4)
RAHMAN, Nelly (RF)

Visitors

Prof SCHICK, Christoph	University of Rostock, Germany, 18 February 2005
Prof MAROM, Gad	The Hebrew University of Jerusalem, Israel, 28 April 2005
Prof BALTA-CALLEJA, J. Francisco	Instituto de Estructura de la Materia, CSIC, Spain, 31 May 2005
Prof SOKOLOV, P. Alexi	University of Akron, United States, 9 September 2005
HONG, Seung In	Korea University, Korea, 1 April - 30 September 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Effect of Charge Density on Phase Separation of Aqueous Solutions of Hetero Polyelectrolytes, Tsubouchi T, Takahashi N, Nishida K, Kanaya T, Annual Meeting, the Society of Polymer Science, Japan, Yokohama, 26 May.

Effect of Ultra-high Molecular Weight Component in Crystallization of Polyethylene under Shear Flow (I) - SAXS Measurments, Sakamoto S, Ogino Y, Matsuba G, Nishida K, Kanaya T, Annual Meeting, the Society of Fiber Science and Technology, Gifu, 9 June.

Structural Analysis of Shish-kebab with X-ray and Neutron Scattering Measurements, Matsuba G, Ogino Y, Nishida K, Kanaya T, 230th ACS National Meeting, Washington DC, USA, 29 August.

Crystallization of Isotactic Polypropylene under Shear Flow -Effect of Shear Rate-, Ogino Y, Matsuba G, Nishida K, Kanaya T, 230th ACS National Meeting, Washington DC, USA, 30 August.

Phase Separation of Hetero Polyelectrolyte Solutions, Nishida K, Tsubouchi T, Kanaya T, 54th Symposium on Macromolecules, Yamagata, 21 September.

Crystallization of Poly(L-lactic acid) , Kawai T, Kanaya T, European Discussion Meeting on Polymer Physics, Polymer Crystallization, Waldau , Germany, 7 October.

Crystallization from Mesomorphic Phase of Isotactic Polypropylene, Konishi T, Nishida K, Matsuba G, Kanaya T, European Discussion Meeting on Polymer Physics, Polymer Crystallization, Waldau , Germany, 7 October.

Neutron Scattering Researches on Soft Condensed Matter, Kanaya T (invited), International Conference on Neutron Scattering, Sydney, Australia, 28 November.

Grants

Kanaya T, Collaboratory on Electron Correlation toward

Phase Inversion in Blend of Aqueous Polyelectrolytes Due to Imbalanced Charge Densities

Most of polymeric materials of different kind or their solutions are difficult to dissolve each other. Even in an exceptional case, such a blend usually shows upper critical solution temperature (UCST) type phase behavior, i.e. the blend is in one phase region and in two phase region above and below the critical temperature, respectively. It is still more rare that the blend shows lower critical solution temperature (LCST) type one, since the entropy loss by demixing in the higher temperature region causes a great penalty for the free energy. We have found that a blend of aqueous solutions of different polyelectrolytes (PSSNa/PVSNa/water) having imbalanced charge densities is a promising system to show the LCST type behavior. When the charge densities of different polyelectrolytes are balanced, normal UCST type behavior is observed. However, as the charge densities of different polyelectrolytes become imbalanced, the phase behavior suddenly changed from the UCST to LCST type (Fig. 1). It is considered that the entropy loss in the higher temperature region is compensated by special repulsive interaction that stabilizes the structure between different polymers.

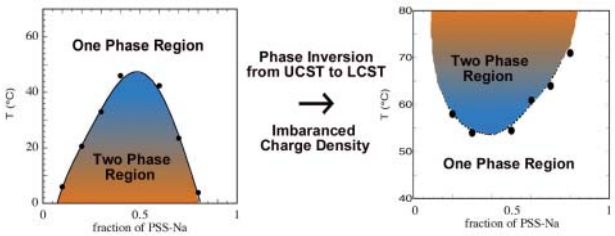


Figure 1. Phase diagrams for blends of aqueous solutions of different polyelectrolytes. Phase inversion occurs when the charge densities of different polyelectrolytes becomes imbalanced.

Crystallization of Poly(L-lactic acid)

Poly (L-lactic acid), PLLA, is one of environmentally friendly polymers that attracted significant interest in recent years. We found novel crystalline form of PLLA (α' phase). In Fig. 2, wide angle X-ray diffraction (WAXD) profiles at higher crystallization temperatures, T_cs, above 120 °C are assigned to be of α-form (10_3 helix, *pseudo-orthorhombic*, a=10.05Å, b=6.1Å, c=28.8Å), while some reflections including (1 0 10) are absent in lower T_cs below 90°C. The results strongly suggest that the disordered α' phase, which has hexagonal lattice (10_3 helix, a=6.2Å, c=28.8Å), is formed at lower temperatures. The disordered α' phase is transformed into the ordered a phase upon heating (Fig. 3). One can see clearly in the WAXD profiles that phase transformation takes place at 150°C. Each reflection shifts to higher q as well as the increase in the number of reflections, which are due to the change in the lattice size and the space group, respectively. The profiles above 150°C were obviously the same as that of high T_c samples (ordered a phase). Moreover, two-step decrease in diffraction intensity has been observed during the melting process. It is reasonable, therefore, to consider that ordered α phase grows through the melting–reorganization or melting–recrystallization mechanism.

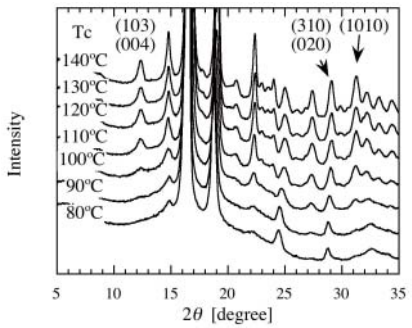


Figure 2. WAXD profiles of PLLA crystallized at various T_cs from the melt.

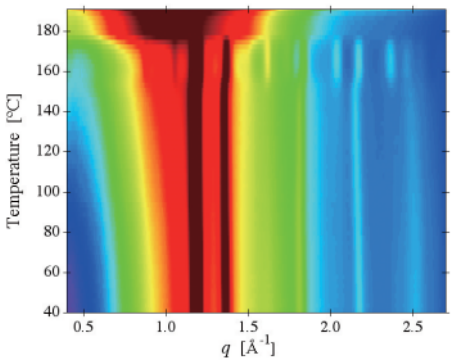


Figure 3. 2D WAXD profiles upon heating at 10°C/min. The sample was pre-crystallized at 80°C.

a New Research Network between Physics and Chemistry, Grand in-Aid for Creative Sientific Research, 1 April 2004 - 31 March 2006.

Kanaya T, Higher Order Structure Formation in Induction Period of PLA Crystallization and in External Fielads, Collaboration Research with Toyota Motor Corporation and Toyota CRDL., INC, 15 January 2003 - 31 March 2006.

Matsuba G, Observation of Shish-kebab Structural Formation Processes of Polymers with Neutron Scattering Technique, Grant-in-Aid for Young Scientists (B), April 2005 - March 2007.

Division of Multidisciplinary Chemistry
- Molecular Rheology -

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

Prof
WATANABE, Hiroshi
(D Sc)

Assoc Prof
INOUE, Tadashi
(D Eng)

Assist Prof
MATSUMIYA, Yumi
(D Eng)

Techn
OKADA, Shinichi

Lecturer (pt)

DEMÉ, Bruno (Ph D) Institut Laue-Langevin, Grenoble, France

Students

OISHI, Yohei (D3)
TAGASHIRA, Masao (M2)
TAKASHIMA, Ryota (M2)
MATSUMOTO, Manabu (M2)
SAWADA, Toshiaki (M1)
NAKATSUJI, Ryo (M1)
KAWANISHI, Yutaka (M1)
MISAWA, Hiroshi (UG)
ICHII, Tomonori (UG)

Scope of Research

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

Research Activities (Year 2005)

Presentations

Detailed Investigation of Entanglement Dynamics with Dielectric and Viscoelastic Methods, Watanabe H, 2nd Annual European Rheology Conference, Grenoble - France, 21 - 23 April.

Rheology of Block Copolymer Micellar Dispersion, Watanabe H, POLYCHAR-13, Singapore (Singapore). 3 - 8 July.

Tube Dilation in Entangled melts: Hierarchical Relaxation and Self-Consistent Coarse-Graining, Watanabe H, 5th International Discussion Meeting on relaxations in Complex Systems: New results, Directions and Opportunities, Lille, France, 7 - 13 July.

Tube Dilation in Entangled melts: A Route of Molecular Description of Viscoelastic Relaxation, Watanabe H, Korea-Australia Rheology Meeting, Cairns (Australia), 17 - 20 July.

Dynamic Birefringence of Cyclic Olefin Copolymers, Inoue T, 4th Pacific Rim Conference on Rheology, Shanghai, China, 8 - 11 August.

Grants

Watanabe H, Grant-in-Aid for Scientific Research (B), Relationship between Loop Content and Rheological Behavior of Multi-block Copolymer System, 1 April 2005 - 31 March 2007.

Inoue T, Grant-in-Aid for Scientific Research (C), Rheology of Surfactant Solution: Nonlinear Elongation and Shear-induced Structure of Thread-like Micelles, 1 April 2005 - 31 March 2007.

Matsumiya Y, Grant-in-Aid for Young Scientists (B), Rheo-dielectric Study on Non-equilibrium Dynamics of Polyether/lithium Salt Mixture Systems, 1 April 2005 - 31 March 2007.

Dynamics of Polybutadienyl Lithium Chains Aggregated in Benzene

In nonpolar solvents, living monoanionic polymer chains having Li as the counter cation aggregate through the association of Li.[1] Experiments have revealed that dimeric and/or tetrameric star-like aggregates are formed as the main component.[1,2] However, dynamics of the aggregates was not elucidated. For this problem, ^{7}Li-NMR and viscosity measurements were conducted for polybutadienyl lithium (PBLi) chains in deuterated benzene (d-Bz) to examine the lifetime τ_{life} and dissociation kinetics of the associated Li domains.[3] The results are summarized below.

Figure 1 compares the viscosity η_{PB} in the living anionic and deactivated states (unfilled and filled symbols) for the PB/d-Bz solutions with the molecular weight M and the concentration C as indicated. At all temperatures T examined, η_{PB} is larger in the living state, demonstrating the aggregate formation of the living PB chains. A separate scattering experiment showed that tetrameric star-like aggregates were formed as the main component.[3]

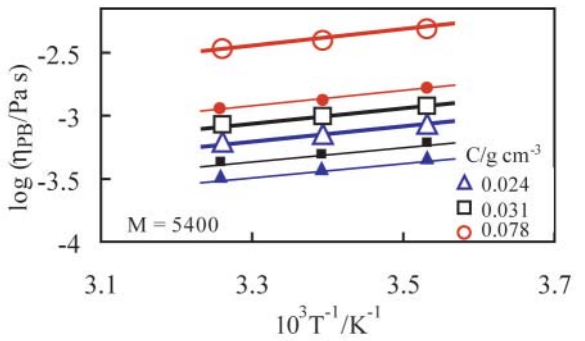


Figure 1. Viscosities of the living and deactivated PB chains (unfilled and filled symbols) with M and C as indicated.

Figure 2 shows the ^{7}Li-NMR spectra of the PBLi/d-Bz solutions with M and C as indicated. The triple peak seen at low T suggests that Li cations are in several different aggregation states and the exchange of these Li species at low T is slow compared to the NMR time scale. With increasing T, this triple peak merges into single peak and thus the exchange becomes faster than the NMR time scale. Analysis of the spectra gave an average lifetime τ_{life} of the Li domain determined by this exchange.[3] In the top panel of Figure 3, τ_{life} for various M and C are plotted against T^{-1}. The Arrhenius behavior is observed for respective M and C, but the magnitude of τ_{life} is strongly dependent on M and C. The origin of these dependencies is discussed below.

Since the activation energy of τ_{life} (≅ 90 kJ mol^{-1}) is considerably lower than the bare Li-Li bond energy[4] (≅ 150 kJ mol^{-1}), the exchange of the Li species should have occurred cooperatively through formation of a larger transient aggregate. This cooperative exchange (occurring at the rate of $1/\tau_{life}$) requires the PBLi tetrameric aggregates to collide each other against an osmotic barrier ΔG_{os}. A time τ_{dif} required for the diffusion over a distance between the aggregates was evaluated from the η_{PB} data (Figure 1), and ΔG_{os} was estimated from the osmotic data in literature.[3] In the bottom panel of Figure 3, τ_{life} for various M and C are normalized by $\tau_{dif}Q_{os}$ ($Q_{os} = \exp(\Delta G_{os}/k_BT)$ with k_B being the Boltzmann constant) and plotted against T^{-1}. The normalized lifetime $\tau_{life}/\tau_{dif}Q_{os}$ is almost universally dependent on T irrespective of M and C. This result demonstrates that the dissociation kinetics of the aggregates is determined by not only the neat Li chemistry but also the polymeric character of the constituent chains reflected in the diffusion time and osmotic barrier.

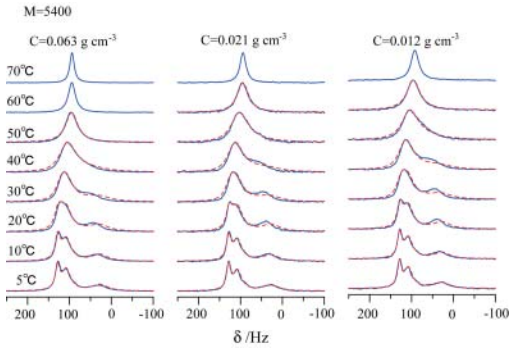


Figure 2. ^{7}Li-NMR spectra obtained for living PB chains with M and C as indicated (solid curves). The dotted curves indicate the spectra reproduced from the analysis.

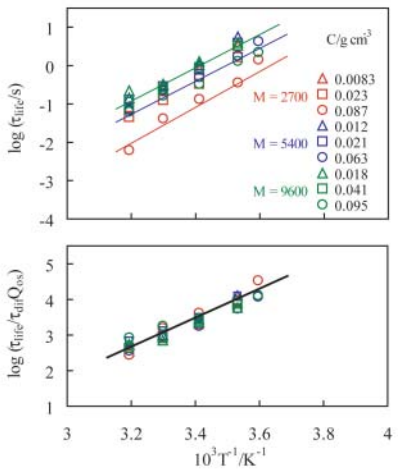


Figure 3. The average lifetime (Li-Li exchange time) τ_{life} for the living PB chains with M and C as indicated. Top and bottom panels indicate the plots of raw τ_{life} data and normalized $\tau_{life}/\tau_{dif}Q_{os}$, respectively.

[1] M. Morton, "Anionic Polymerization: Principles and Practice", Academic Press, New York, 1983.
[2] A. Z. Niu et al., *J. Chem.* Phys., **122**, 134906 (2005).
[3] Y. Oishi et al., *Polymer J.*, in press.
[4] A. Frischknecht and S. T. Milner, *J. Chem. Phys.*, **114**, 1032 (2001).

Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

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

Prof
SATO, Naoki
(D Sc)

Assoc Prof
ASAMI, Koji
(D Sc)

Assist Prof
KITA, Yasuo
(D Sc)

Assist Prof
YOSHIDA, Hiroyuki
(D Sc)

Guest Res Assoc
MURDEY, Richard James
(Ph D)

A Res
KATOH, Keiichi
(D Sc)

Students

HIRAMATSU, Takaaki (D3)
TSUTSUMI, Jun'ya (D3)
ARAKAWA, Naofumi (M2)
WATAZU, Yuji (M2)
MORIE, Jun (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, biopolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2005)

Presentations

Simulation of Dielectric Relaxation in Biological Cells of Arbitrary Shape (in Japanese), Asami K, The 27th Annual Meeting of the Membrane Society of Japan (Tokyo, Japan), 19 - 20 May.

Frontier Electronic Structures in Organic Semiconductor Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies, Sato N, Murdey R J, The 3rd Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (ASOMEA III) (Vadstena, Sweden), 2 - 5 June.

Frontier Electronic Structure of Fluorinated Copper Phthalocyanine Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies, Murdey R, Bouvet M, Sato N, The 54th Fujihara Seminar: Organic Semiconductors and Conductors - Half Century and Future Prospects (OSCC50) (Tomakomai, Japan), 31 August - 4 September.

Contribution of Electronic Polarization to Electrostatic Lattice Energy in Organic Molecular Crystals (in Japanese), Tsutsumi J, Kato S, Sato N, The 14th Organic Crystals Symposium (Kyoto, Japan), 30 September - 1 October.

Evaporation of Aluminum Clusters on Organic Semiconductor Thin Films (in Japanese), Yoshida H, Sato N, Bunshi-kozo Sogo Toronkai (Symposium on Molecular Structures and the Related Problems) 2005 (Tokyo, Japan), 27 - 30 September.

Dielectric Dispersion of Lysed Erythrocytes (in Japanese), Asami K, The 43rd Annual Meeting of the Biophysical Society of Japan (Sapporo, Japan), 23 - 25 November.

Grants

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

Yoshida H, Controlling Reactivity and Diffusion at

Frontier Electronic Structures in Fluorinated Copper Phthalocyanine Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies

Copper phthalocyanine [CuPc] and the fluorinated analog [Cu(F_{16}Pc)] are very different materials from the standpoint of their electronic properties. CuPc is a hole transport material, typical of organic semiconductors. In contrast Cu(F_{16}Pc) is one of the few air-stable compounds known to exhibit electron transport, characteristics that make it of considerable interest in the development of molecular electronic devices. In an recent example, an ambipolar transistor has been demonstrated using thin layers of pure, undoped CuPc and Cu(F_{16}Pc) as the p-type and n-type semiconductors, respectively.

We have examined the effect of fluorine substitution on the electronic structure of phthalocyanines, with particular attention paid to the states near the HOMO-LUMO gap. Unoccupied states were directly observed with inverse photoemission spectroscopy (IPES), while the corresponding measurement on occupied states was performed with ultraviolet photoelectron spectroscopy (UPS).

Thin films of CuPc, a partially fluorinated intermediate compound Cu(F_8Pc), and Cu(F_{16}Pc) were prepared by vacuum deposition on clean gold substrates. Spectra were taken in-situ under UHV conditions. As seen in Fig. 1, the results show that while the transport energy gap remains almost constant at about 2 eV, there is a readily apparent, rigid shift of the gap to higher binding energies with increasing fluorine substitution. The charge injection barrier heights stay essentially unchanged, however, as the substrate Fermi level is pinned near the middle of the phthalocyanine HOMO-LUMO gap in all three systems. This work was carried out in collaboration with Prof. Marcel Bouvet at Laboratoire de Chimie Inorganique et Matériaux Moléculaires, CNRS, France.

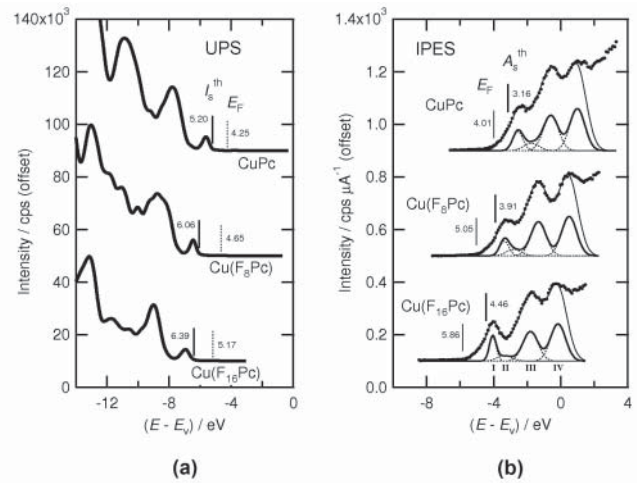


Figure 1. (a) UPS and (b) IPES spectra of 8 nm-thick CuPc, Cu(F_8Pc) and Cu(F_{16}Pc) films on gold substrates. The energy scale is plotted against the vacuum level of the organic film. Gaussian fits are shown for the IPES spectra, compensated for the resolution of the instrument. Determined energy positions are indicated by vertical bars with respective values.

Numerical Simulations of Dielectric Dispersion in Biological Cells of Complex Geometry

Biological cells show dielectric dispersion due to interfacial polarization, i.e., accumulation of charges at the membrane interfaces by the applied electric field. For cells of simple geometry, we have used analytical approaches for analyzing the dielectric dispersion. However, it is difficult to derive analytical formulas for cell models of complex geometry. Hence, a numerical technique based on the three-dimensional finite difference method has been developed to calculate the equivalent complex permittivity of a system including a single cell or periodically arranged cells in a continuous medium. The numerical method successfully simulated dielectric dispersion of cells in cell division, i.e., a spherical cell divides into two spherical cells via a doublet-shaped cell with a narrow cytoplasmic junction. Further, it has uncovered the underlining mechanism of the α-dispersion of osmotically-lysed erythrocytes, which has remained open since its finding in 1957. The α-dispersion is caused by formation of a single hole of several tens nm in radius in the plasma membrane.

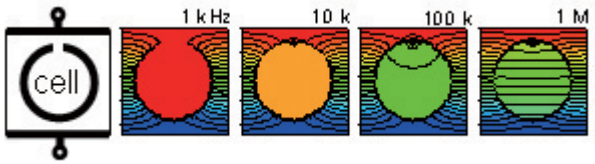


Figure 2. Electrical potential distributions in a cell model with a hole.

Metal-Organic Semiconductor Interfaces through the Deposition of Metal Clusters, Grant-in-Aid for Scientific Research for Young Scientists (B), 19 October 2004 - 31 March 2006.

Division of Multidisciplinary Chemistry
- Supramolecular Biology -

http://www.scl.kyoto-u.ac.jp/~umeda/index.htm

Prof
UMEDA, Masato
(D Pharm Sc)

Assist Prof
TAKEUCHI, Ken-ichi
(D Pharm Sc)

Assist Prof
KATO, Utako
(D Sc)

Res Associate
INADOME, Hironori
(D Agr)

PD
SHISHIOH, Nobue
(D Med Sc)

PD (JSPS)
HAMASAKI, Maho
(D Sc)

Res Associates (pt)

YAMAGUCHI, Yukiko
NISHIKAWA, Miwako

Students

TAKAHARA, Keigo (D2)
TANIUCHI, Kentaro (D1)
SUGATANI, Tatsushi (RS)

Scope of Research

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

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

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

Research Activities (Year 2005)

Presentations

Lipid Field in Biological Membranes. Umeda M. JST Workshop. 23 - 24 March, Hamamatsu.

Mass Spectrometry of Phospholipids Using an Intense Femtosecond Laser. Kato U., Shimizu S., Taniuchi K., Sakabe S., Umeda M. The 47th Japanese Conference on the Biochemistry of Lipids, 2 - 3 Jun, Kanazawa.

A New Approach for Molecular Lipid Biology Using Drosophila. Umeda M. Japanese Drosophila Research Conference. 7 - 9 July, Awaji.

Membrane Lipids and Cell Size Control. Umeda M., Taniuchi K., Inadome H., Shishioh N., Kato U. The 78th Annual Meeting of The Japanese Biochemical Society. 19 - 22 October, Kobe.

Regulation of Actin Filament Assembly by Dynamic Redistribution of Plasma Membrane Phosphatidy Lethanolamine. Inadome H., Emoto K., Umeda M. The 78th Annual Meeting of the Japanese Biochemical Society. 19 - 22 October, Kobe.

Generation of the Hypomorphic Allele of Stearoyl-CoA Desaturase in *Drosophila*. Takahara K., Takeuchi K., Yamamoto D., Umeda M. The 78th Annual Meeting of the Japanese Biochemical Society. 19 - 22 October, Kobe.

Membrane Lipid Dynamics and Cellular Morphogenesis. Umeda M., Taniuchi K., Inadome H., Shishioh N., Kato U. The 43rd Annual Meeting of The Biophysical Society of Japan. 23 - 25 November, Sapporo.

Grants

Umeda M, Cellular Morphogenesis Based on the Positional Information of Membrane Phospholipids. Grant-in-Aid for Scientific Research (A)(2), 1 April 2003 - 31 March 2007.

Umeda M, Identification of Genes Involved in Thermo-

Regulation of Membrane Phospholipid Dynamics and Its Role in Cell Morphogenesis

Biological membranes consist of a phospholipid bilayer where phospholipid molecules move not only laterally but also across the two layers of the bilayer membranes. Although it is generally believed that the organized movements of membrane phospholipids play a pivotal role in regulating the structure of biomembranes, the molecular mechanisms underlying the controlled movements of membrane phospholipids are still poorly understood. To identify the molecules that regulate the movements of membrane phospholipids, we have isolated a series of yeast mutants with disordered organization of membrane phospholipids. By analyzing the genes defective in these mutants, we have identified a novel membrane protein, Ros3p, which is required for the translocation of phospholipids across the yeast plasma membrane. Ros3p is highly conserved among various organisms including worm, fly and mammals, implicating a general role for cellular functions. To reveal the biological functions of ROS3 family proteins, we have established a series of mutant flies in which the expression level of ROS3 protein is genetically manipulated. We found that the reduced expression of ROS3 protein caused marked reduction in the size of cells during larval development (Figure.1a). Overproduction of ROS3 protein resulted in increased cell size and disorganized organ structure (Figure.1b). These results suggest that ROS3 family proteins play a role in controlling the size and morphology of cells through regulating the movement of membrane phospholipids.

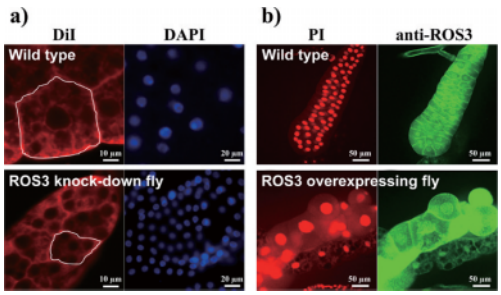


Figure 1. Changes in the expression of ROS3 proteins caused abnormal cell size and organ structure during larval development of *Drosophila*.
a) Fat body cells in the wild type and the ROS3 knock-down flies were stained with a lipophilic dye (DiI) and a nucleic marker (DAPI). Each cell was framed in a white line.
b) Salivary gland cells in the wild type and the ROS3 overexpressing flies were stained with anti-ROS3 antibody and a nucleic marker (PI).

The Molecular Mechanisms of Thermoregulation in Animals: The Role of Dystroglycan in Determination of the Thermoregulatory Set Point in Drosophila

Temperature is a critical variable with a profound impact on living organisms. A wide variety of animals sense the environmental temperature, move toward to thermally comfortable zone, and tend to remain for relatively long periods. The tendency to remain still in this preferred range may be regarded as a mechanism to keep the animals within a range of temperatures, namely the thermoregulatory set point, which is optimal for most physiological metabolic processes. Moreover the preferred temperature differs among species as well as among individuals within a species. Progress has been made in the identification of molecules involved in the sensation of peripheral temperature, but the molecular mechanisms that determine the thermoregulatory set point remain poorly understood. In an effort to identify genes involved in temperature preference, we searched for mutations that affect temperature preference of *Drosophila melanogaster*, and identified the *atsugari* mutant, which shows a preference for unusually low temperature. We showed that the *atsugari* phenotype was caused by the reduced expression of dystroglycan. We also found that the *atsugari* mutant exhibited a striking tolerance to cold temperature (Figure2). These results suggest that the defective expression of dystroglycan in the *atsugari* mutant results in downward resetting of the thermoregulatory set point as well as the lower limit of cold tolerance. Although dystroglycan has been characterized as a central molecule involved in the pathogenesis of muscular dystrophy, our studies revealed a novel role for dystroglycan in thermoregulatory functions of animals.

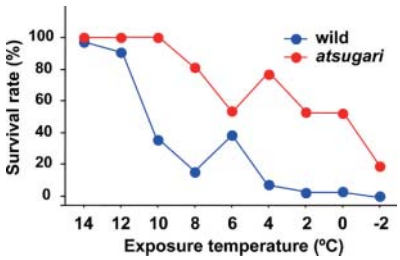


Figure 2. The *atsugari* mutant showed a striking tolerance to cold temperatures. Third-instar larvae of the *atsugari* mutant and wild type were exposed to cold temperatures under constant darkness for 24 h. After exposure, they were placed at 25°C for 48 h and checked for survival.

regulatory Behavior of Insects. Special Cooperation Funds for Promoting Science and Technology from the MEXT Agency of Japan. 1 April 2002 - 31 March 2006.

Takeuchi K, Development of a New *Drosophila* Model for Studying Muscular Dystrophy. Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2007.

Inadome H, Analysis of the Asymmetric Distribution of the Phospholipids in the Golgi Apparatus in Yeast. Grant-in-Aid for Scientific Research for Young Scientists (B), 1 April 2005 - 31 March 2007.

Advanced Research Center for Beam Science
- Particle Beam Science -

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

Prof
NODA, Akira
(D Sc)

Assoc Prof
IWASHITA, Yoshihisa
(D Sc)

Assist Prof
SHIRAI, Toshiyuki

Techn
TONGU, Hiromu

PD
IKEGAMI, Masahiro
(D Sc)

Students

NAKAMURA, Shu (D3)
YAMAZAKI, Atsushi (D3)
FUJIMOTO, Shinji (D3)
MIHARA, Takanori (D2)
TANABE, Mikio (D1)
ITOH, Hiroyuki (M2)
SOUDA, Hikaru (M2)
SHINTAKU, Hiroki (M1)

Visitors

Prof HOFMANN, Ingo	GSI, Germany, 2 March 2005
Prof HANGST, Jeffrey	University of Aarhus, Denmark, 17 March 2005
Dr COUPRIE, Marie-Emmanuelle	LURE, France, 24 October 2005
Prof SHEVELKO, V.P.	Lebedev Physical Institute, Russia, 26 October 2005
Prof SYRESIN, Evgeny	JINR, Russia, 16 November - 1 December 2005
Dr SELEZNEV, Igor	JINR, Russia, 21 November - 8 December 2005

Scope of Research

Particle and photon beams generated with accelerators and their instrumentations both for fundamental research and practical applications are studied. 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: Radiation mechanism of photons by electrons in the magnetic field: R&D to realize a compact synchrotron dedicated for cancer therapy; and Irradiation of materials with particle and photon beams.

Research Activities (Year 2005)

Presentations

Approach to Crystalline Beam at S-LSR with Use of the Electrostatic Potential Combined with the Magnetic Field, Noda A, First International Workshop on Electrostatic Storage Devices, Israel, 2 June 2005.

Beam Simulations in S-shaped Curved Solenoids, Iwashita Y, 7th International Workshop on Neutrino Factories and Superbeams, Italy, 22 June 2005.

Phase Rotation Scheme of Laser Produced Ions for Reduction of the Energy Spread, Noda A, Nakamura S, Iwashita Y, Sakabe S, Hashida M, Shirai T, Shimizu S, Tongu H, Ito H, Souda H, Yamazaki A, Tanabe M, 14th International Laser Physics Workshop, Japan, 7 July 2005.

RF Kicker Update, Iwashita Y, 2005 International Linear Collider Physics and Detector Workshop and Second ILC Accelerator Workshop, USA, 18 August 2005.

Experimental Study of Dispersion Control Utilizing both Magnetic and Electric Fields, Tanabe M, Ikegami M, Noda A, Shirai T, Souda H, Tongu H, Shibuya S, Noda K, The International Workshop on Beam Cooling and Related Topics, USA, 19 September 2005.

Laser Cooling for 3-D Crystalline State at S-LSR, Noda A, Fujimoto S, Ikegami M, Shirai T, Souda H, Tanabe M, Tongu H, Shibuya S, Takeuchi T, Okamoto H, Grieser M, Noda K, The International Workshop on Beam Cooling and Related Topics, USA, 23 September 2005.

Development of Final Focus Permanent Magnet, Mihara T, Iwashita Y, Kumada M, Workshop on Nano Scale Beams (Nanobeam 2005), Japan, 18 October 2005.

Commissioning of S-LSR, Shirai T, Noda A, Fujimoto S, Ikegami M, Souda H, Tanabe M, Tongu H, Shibuya S, Takeuchi T, Fujimoto T, Iwata S, Okamoto H, Grieser M, Noda K, Workshop on Nano Scale Beams (Nanobeam 2005), Japan, 20 October 2005.

Beam Monitoring System and Orbit Correction in S-LSR, Fujimoto S, Noda A, Ikegami M, Souda H, Tanabe M, Tongu H, Shirai T, Takeuchi T, Noda K, Workshop on Nano Scale Beams (Nanobeam 2005), Japan, 20 October 2005.

Beam Commissioning and First Electron Beam Cooling at S-LSR

The ion storage and cooler ring, S-LSR have been constructed at Institute for Chemical Research (see Figure 1). The beam commissioning was started from the beginning of October, 2005. The linac injected the 7 MeV proton beam into the new ring. We observed the first beam accumulation at 10th October. The number of the accumulated proton was $3x10^7$ particles. Now it is improved up to 10^9 particles.

The aim of S-LSR is technical developments of the compact ion accelerator for the cancer therapy using the electron beam cooling. The commissioning of the electron beam cooler was started from 31st October. Figure 2 shows the results of the first cooling experiments. We succeeded in reducing the horizontal beam size from 40mm to 1mm and the momentum spread from 0.4% to 0.02% without any beam losses. As a result, the beam density in the phase space is increased about 10^6 times higher.

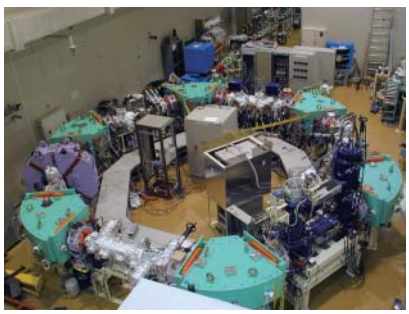


Figure 1. View of the ion storage / cooler ring, S-LSR.

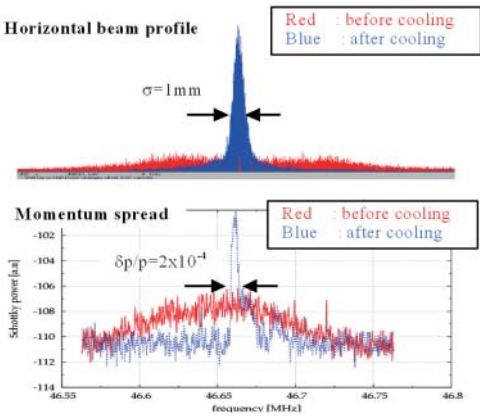


Figure 2. Measured beam profile and the momentum spread before and after cooling. They are measured by the MCP and Schottky monitor.

Phase Rotation of the Laser Produced Ions

Recently there are many reports of the high energy ion production by high intensity, ultra short pulse lasers. The energy spread of the laser produced ions is very wide from 0 to 100% without the energy peak. This situation can be greatly improved using the phase rotation scheme by the RF field synchronized with the laser pulse.

The phase rotation experiment was carried out at JAEA-KANSAI. Figure 3 shows the RF cavity for the phase rotation. The laser pulse up to 4 TW, 70 fsec was focused on the Ti foil with the thickness of 3 μm. The laser field is about 10^{18} W/cm^2 on the target. Figure 4 shows the energy spectrum of the laser produced ions. There is no energy peak without the phase rotation. With the phase rotation, the energy peaks appears when the ion energy matches the phase of the RF field.

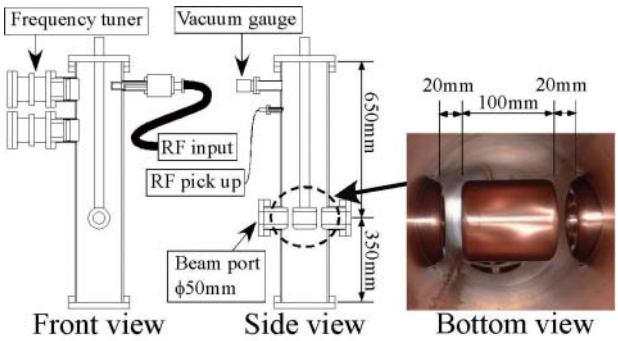


Figure 3. View of the phase rotation cavity.

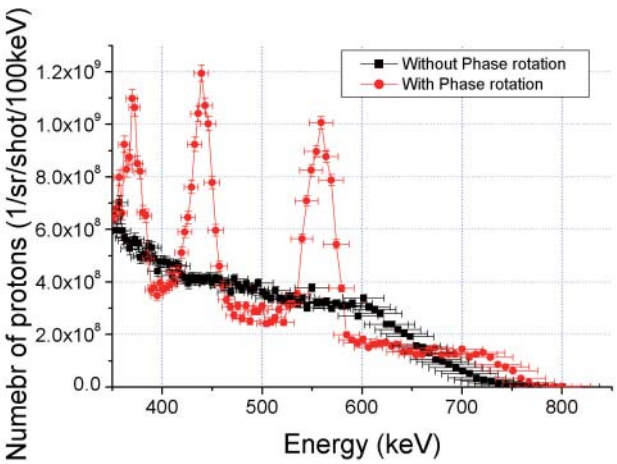


Figure 4. Energy spectrum of the laser produced ions with and without the phase rotation.

Grants

Noda A, Beam Accumulation and Cooler Ring, Advanced Compact Accelerator Research, April 2001 - March 2006.

Iwashita Y, Super Strong Permanent Magnet for Final Focus Lens in Linear Collider, Grant-in-Aid for Scientific Research, (A) (1), April 2002 - March 2006.

Shirai T, High Energy Electron Extraction from Electron Storage Ring, Grant-in-Aid for Scientific Research, (C) (2), April 2004 - March 2006.

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

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

Prof
SAKABE, Shuji
(D Eng)

Assist Prof
HASHIDA, Masaki
(D Eng)

Assist Prof
SHIMIZU, Seiji
(D Sc)

Students

SHIRAI, Kouta (M2)
MASUNO, Shinichiro (M1)

Scope of Research

By making the physics of interaction between femto-second laser and matters clear, possibility for new applications is being developed in such as laser processing and laser nuclear science. The interaction of femto-second laser and matter differs from that of nanosecond laser in physics such as ionization and ablation process. Soft-ionization and ablation by the femto-second laser (we named it nano-ablation) can be applied to mass spectrometry and nano-scale structural formation and matter reforming, respectively. In addition, with the progress of short pulse lasers, even a small-sized equipment can create ultra-high optical field. In this strong electromagnetic field the motion of an electron becomes relativistic, and the electron is accelerated easily above MeV, emitting high energy pulse x-rays and ions. Laser produced radiation has the feature such as impulse, a point source and high intensity, and its potential to the new radiation source is expected. In our laboratory physics of intense laser matter interactions and its application are researched.

Research Activities (Year 2005)

Presentations

Energetic Ion Generation by Coulomb-explosion in Cluster Gas and a Low-density Plastic Foam with an Intense Femtosecond Laser, Sakabe S, International Symposium on Atoms, Molecules, and Clusters in Intense Laser Fields 2, 24 - 25 January 2005.

Desorption/ionization of Coronene and C_{60} Molecules Irradiated by an Intense Short-pulse Laser, Shimizu S, Hashida M, Sakabe S, International Symposium on Atoms, Molecules, and Clusters in Intense Laser Fields 2, 23 - 24 January 2005.

Intense Short-pulse Laser Application Research at Institute for Chemical Research, Kyoto University, Sakabe S, Korea-China-Japan Workshop on Ultrashort High-Intensity Laser Development and Their Applications, 21 - 22 March 2005.

Energetic Ion Generation by Coulomb-explosion in Cluster Gas and a Low-density Plastic Foam with an Intense Femtosecond Laser, Sakabe S, Hashida M, and Shimizu S, Advanced Lasers and their Applications, 12 - 14 May 2005.

Study of Fast Electron Transport in Hot Dense Matter Using X-ray Spectroscopy, Nishimura H, Inubushi Y, Ochiai M, Fujioka S, Kawamura T, Hashida M, Simizu S, Sakabe S, et. al., 32nd EPS Plasma Physics Conference and 8th International Workshop on Fast Ignition of Fusion Targets, 27 June - 1 July, 2005.

Nanostructure Formation on Metals by Femtosecond Laser Pulses, Hashida M, Shimizu S, and Sakabe S, 14th International Laser Physics Workshop, 4 - 8 July 2005 (Invited).

Energetic Ion Generation by Coulomb-explosion in Cluster Gas and a Low-density Plastic Foam with an Intense Femtosecond Laser, Sakabe S, Hashida M, and Shimizu S, 14th International Laser Physics Workshop, 4 - 8 July 2005 (Invited).

Periodic Nano Structure Formation on Metals by Femtosecond Laser Pulses, Hashida M, Shimizu S, and Sakabe S, International Workshop on Intense Laser-Matter Interaction and Pulse Propagation, 15 - 19 August 2005.

Desorption/ionization of Organic Molecules Irradiated by an Intense Laser, Shimizu S, International Workshop on Intense Laser-Matter Interaction and Pulse Propagation, 15 - 19 August 2005.

Carbon Nanotubes Cathode Modified by Femtosecond Laser Ablation, Hashida M, Shimizu S, and Sakabe S, 8th Conference on Laser Ablation, 11-16 September 2005.

Grants

Sakabe S, Research on Coulomb Explosion Dynamics of Cluster Molecules with Intense Lasers, Grant-in-Aid for Scientific Research (B)(2), 1 April 2003 - 31 March 2006.

Hashida M, Advanced Material Processing with Femtosecond Lasers, Grant-in-Aid for Young Scientists (B), 1 April 2005 - 31 March 2007.

Completion of Intense Femto-second Laser System T⁶-laser for the Research of Laser-matter Interaction and Its Applications

Ultra intense femtosecond laser system T⁶ (the acronym of Table-top Ten TW Ten Hz Tunable Ti:sapphire) laser has been installed in the new laser building, which was completed in 2004, adjacent to the building of accelerator facility. The system is a Ti:sapphire chirped-pulse amplifier laser, delivering 1J (at maximum), 100fs pulses at a center wavelength of 800nm and repetition rate variable from single shot to 10Hz at maximum. The laser has been successfully operated in the laser building constructed for less mechanical vibration on the floor against earthquake and high stability of temperature and humidity controls. Since the first experiment for laser nano-ablation, we have been doing the experiments of laser processing, soft ionization, laser produced radiations, and collaboration research with ICR, another university. The laser and irradiation systems are continuously improved for more efficient collaboration research, and will be opened for the researcher with our common interests.

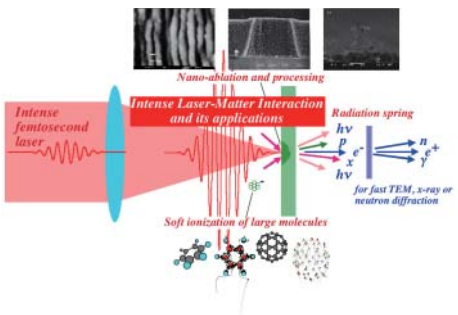


Figure 1. Intense femtosecond laser-matter interaction physics and its applications.

Ultrashort-Pulse Laser Ablation of Fluoropolymer

Laser -ablation experiments were performed on polytetrafluoroethyhlene (PTFE) with femtosecond Ti:sapphire pulse laser. The released ions upon ablation were detected by time of flight mass spectrometer (TOF-MS) with 130fs and 400ps pulse laser. The difference was shown in detected ions and laser fluence dependence of them between two pulses. The ablation threshold of PTFE was also investigated from the crater surface diameter dependence on the laser fluence. It was found that the ablation threshold was approximately proportional to pulse duration to the power 0.39 in the range of 130fs-400ps. It was suggested that the ablation of organic polymer material such as PTFE might be controlled by the mechanism different from multiphoton absorption.

Carbon-nanotubes Cathode Modified by Femtsecond Laser Ablation

Femtosecond laser ablation of the carbon nanotubes (CNTs) cathode was demonstrated in the laser fluence range of 0.05-2J/cm^2. It was shown that the CNTs were aligned perpendicular to the cathode surface by the laser ablation. The emission characteristics of the CNTs cathode were measured by a diode system. The modified CNTs cathode turned on electron emission at the electric field of 1.8V/μm, which was approximately half of original CNTs cathode and the 10% lower than that of nanosecond laser ablation. As the laser fluence decreased, the electric field of turn-on had the tendency to be lower.

Elements and Their Transitions Feasible for NEET

Electron and nuclear transitions in the nuclear excitation by electron transition (NEET) process have been investigated. The NEET transitions for nuclei are presented in a table in which the electron and nuclear transitions, their transition energies, transition multipoles, and nuclear spin angular momentum are given. The elements are listed for which the difference between the electron and nuclear transition energy is <5 keV, because the NEET probability will be appreciable if the electron transition energy is close to the nuclear transition one. As both the experimental and theoretical studies for NEET are at an early stage, only the elements and their parameters related to NEET are listed here. The present compilation, however, provides a useful direction for future studies of NEET and its applications to nuclear science.

Desorption/ionization of Bio-molecules with Intense Femtosecond Laser

Desorption/ionization of bio-molecules with intense femtosecond laser (800nm wavelength, 130 fs pulse duration) was studied by-means-of time-of-flight mass spectrometry. The molecular ions of some lipid molecules were observed at the laser intensity around the ionization thresholds. The signal intensity of the molecular ion and fragment ions increase with increasing the laser intensity. The laser intensity dependence of the signal intensity for the observed ions suggested that ionization mechanism might be non-resonant multiphoton ionization. The desorption/ionization by non-resonant multiphoton ionization will have a great possibility as a new soft-ionization method.

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

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

Prof
ISODA, Seiji
(D Sc)

Assoc Prof
KURATA, Hiroki
(D Sc)

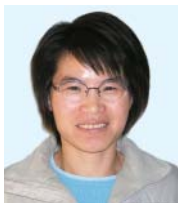
Assist Prof
OGAWA, Tetsuya
(D Sc)

Assist Prof
NEMOTO, Takashi
(D Sc)

Res Associate
MORIGUCHI, Sakumi
(D Sc)

Res
YOSHIDA, Kaname
(D Sc)

Res
TSUJIMOTO, Masahiko



Res
JIU, Jinting
(D Eng)

A Res
YAJI, Toyonari
(D Sc)

A Res
KUWAMOTO, Kiyoshi

Students

MINARI, Takeo (D3)
MIYAMOTO, Yusuke (D3)
KIYOMURA, Tsutomu (D1)
HARUTA, Mitsutaka (M2)
NAGAMATSU, Daiki (M2)
ISOJIMA, Seiichi (M1)

Visitors

Dr MAGONOV, Sergei	Digital Instruments/Veeco Metrology, USA, 15 July 2005
Prof WANG, Hao	Beijing University of Technology, China, 26 July 2005
Dr FRANCO, Olga	Universidad Complutense, Spain, 1 - 21 August 2005
Prof CHOU, Li-Jen	National Tsing-Hua University, Taiwan, 1 September 2005 - 31 March 2006

Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. It aims to explore new methods for imaging and also obtaining chemical information in thin films, nano-clusters, interfaces, and even in solutions. By combining this with scanning probe microscopy, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, fabrication of low-dimensional functional assemblies.

Research Activities (Year 2005)

Presentations

Single-grain Organic Field-effect Transistors Based on Pentacene Thin Film Phase, Minari T, Nemoto T, Isoda S, The 5th International Conference on Electroluminescence of Organic Materials and Related Phenomena, 17 - 21 January, Phoenix USA.

Core-hole Effects on Oxygen K-ELNES of Transition Metal Oxides, Kurata H, Tsujimoto M, Nomoto T, Isoda S, International EELS Workshop EDGE 2005, 1 - 5 May, Grundlsee, Austria.

Organic Field-effect Transistors Based on Thienyl-Furan Oligomers, Minari T, Terayama M, Miyata Y, *et al*., 8th European Conference on Molecular Electronics, 29 June-3 July, Bologna, Italy.

STM and STS Studies on Platinum Chains in Bis(1,2-benzoquinonedioximato)platinum, Yaji T, Yoshida K, Tsujimoto M, Nemoto T, Kurata H, Isoda S, KJF 2005, 26 - 29 October, Daejeon, Korea.

Polymorphs of Ni(salen) Grown on Substrates, Yoshida K, Isoda S, The 2005 International Chemical Congress of Pacific Basin Societies, 15 - 20 December, Hawaii, USA.

Structural Analysis of Bis (1,2-benzoquinonedioximato)platinum(II) Polymorphs Formed Epitaxially on Alkali Halides

We analyzed the crystal structures of bis(1,2-benzoquinonedioximato)platinum(II), ($Pt(bqd)_2$), thin films fabricated by vacuum deposition on the (001) surfaces of NaCl, KCl, KBr and KI substrates at room temperature. $Pt(bqd)_2$ thin films exhibited some polymorphs. These structures and crystallographic orientations were studied by transmission electron microscopy (TEM). On NaCl, KCl and KBr, $Pt(bqd)_2$ grows in the β-form; unit cell dimensions are a=2.57 nm, b=0.66 nm and c=0.37 nm. The β-polymorph transforms into the ordinary orthorhombic α-form by heating at different rates depending on the substrate. The instability of the β-form was influenced by lattice-matching between the β-form and substrate used. On KI, $Pt(bqd)_2$ grows as another polymorphic tetragonal form (γ-form: a=1.42 nm and c=0.656 nm). From the result of high-resolution TEM observations, many defects or domain boundaries in this film were observed, which are related to the structural change during the growth.

Yoshida K *et al., JJAP*, **44**(1B), 491-494 (2005).

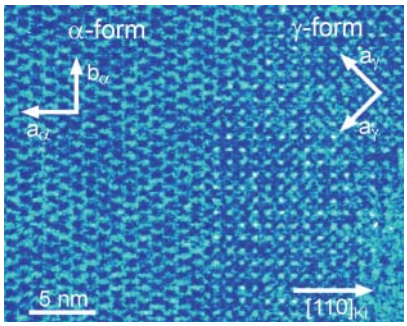


Figure 1. HRTEM image of the interface between the α- and γ-forms.

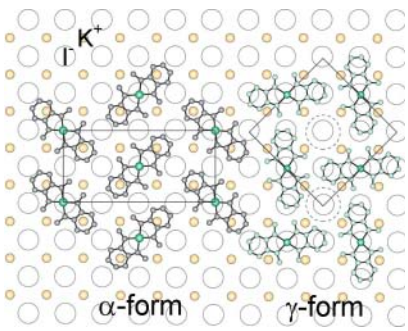


Figure 2. Model of interface between α-form and γ-form on KI substrate.

Influence of Nitrogen Vacancies on the N K-ELNES Spectrum of Titanium Nitride

We have calculated the nitrogen K-ELNES of TiN_x including N vacancies by the first-principles band calculations (WIEN2K). It has been demonstrated that the change of ELNES due to the vacancy depends on the atomic configuration between the vacancy site and the excited atom. The influence of vacancy appears to be strong when the vacancy occurs at the second nearest neighbor site from the excited atom. The vacancy levels, mainly consisting of Ti d states at first nearest neighbor site, are found to occur ~-2 eV and near the Fermi level. These levels reduce the intensity of the N p-DOS at the top of the conduction band on account of the hybridization between Ti d and N p states, which causes the decrease of energy separation between the relevant peaks observed in experimental ELNES spectra. The calculated spectra agree fairly well with the experimental ones, although a supercell of considerably larger size than that afforded by the computational powers available in this study is needed to simulate composition-induced changes in calculated ELNES spectra.

Tsujimoto M *et al*., J. *Electron Spectrosc. Relat. Phenom*., **143**, 159-165 (2005).

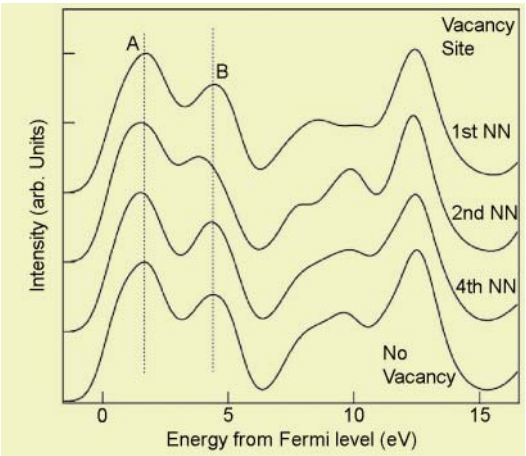


Figure 3. Site-resolved N K-ELNES for $TiN_{0.97}$ involving a vacancy at different distances from the excited atom.

Grants

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

Kurata H, Local State Analysis of Organic Materials by Spatially and Angular Resolved EELS, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2006.

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2005 - 31 March 2006.

Advanced Research Center for Beam Science
- Structural Molecular Biology -

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

Prof
HATA, Yasuo
(D Sc)

Assoc Prof
ITO, Yoshiaki
(D Sc)

Assist Prof
FUJII, Tomomi
(D Sc)

Res
TOCHIO, Tatsunori
(D Sc)

Students

OoHASHI, Hirofumi (D3)
SAKAKURA, Shusuke (D1)
MIZOTA, Hirohisa (D1)
HORIGUCHI, Daisuke (M2)
YOKOI, Koji (M2)
GODA, Yuko (M1)

Scope of Research

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

Research Activities (Year 2005)

Presentations

Structure and Inhibition Mode of Protein I^C in Complex with Carboxypeptidase Y, Hata Y, Hayashida M, Fujii T *et al*., XX Congress of the IUCr, 30 August.

The Structure of Carboxypeptidase Y Inhibitor I^C in Complex with the Cognate Proteinase and a Novel Mode of the Proteinase-Protein Inhibitor Interaction, Hata Y, Hayashida M, Fujii T *et al*., Pacifichem2005, 16 December.

Structure of the Carboxypeptidase Y Inhibitor I^C in Complex with the Cognate Proteinase Reveals a Novel Mode of the Preteinase-Protein Inhibitor Interaction, Mima J (Kyoto University), Hayashida M, Fujii T *et al*., J. Mol. Biol. **346**, 1323-1334 (2005).

Structure and Inhibition Mode of Protein I^C in Complex with Carboxypeptidase Y, Hata Y, Hayashida M, Fujii T *et al*., Acta Cryst. **A61** (Supplement), C190 (2005).

Grants

Hata Y, Structural Analyses of Gene-products Involved in Protein Structure Formation, Protein 3000 Project, 1 April 2002 - 31 March 2007.

Sanjoh A (Protein Wave Corporation), Hata Y *et al*., Studies and Developments on Practical Use of Devices for Growth of Protein Crystals Suitable for Ultra-high Resolution X-ray Analysis, Grant for Support of Studies and Developments by Cooperation of Industry, Academic and Public, Kyoto Sangyo 21 Foundation, 1 April 2004 - 31 March 2006.

Ito Y, Development of Basic Technologies for New Functional Particle Materials, Kyoto Prefecture Collaboration of Regional Entities for the Advancement of Technological Excellence, JST, 2004 - 2008.

Crystal Structure of the Inhibitor I^C in Complex with Carboxypeptidase Y

The proteinous proteinase inhibitor I^C, which exists in the cytoplasm of the yeast *Saccharomyces cerevisiae*, specifically forms the 1:1 complex with and then inhibits carboxypeptidase Y (CPY) which is the vacuolar serine carboxypeptidase. The inhibitor belongs to the phosphatidylethanolamine-binding protein (PEBP) family. In order to reveal the inhibitory mode of I^C against CPY, we determined the 2.7Å crystal structure of the I^C-CPY complex by the MR method of X-ray crystallography. This represents the first structure of a natural serine carboxypeptidase inhibitor complexed with the cognate proteinase and also that of a PEBP member complexed with its macromolecular binding partner.

The final structure model of the I^C-CPY complex contains 204 amino acid residues of I^C consisting of 219 amino acid residues. Residues Lys73-Ala78 and Glu122-Ala130 of I^C are excluded in the model because they are invisible in the electron density map. The overall structure of the complex is a compact ellipsoidal structure (Fig1). The structure of the complex contains two binding sites of I^C toward CPY: the N-terminal inhibitory reactive site and the secondary CPY-binding site, which interact with the S1 substrate-binding site of CPY and the hydrophobic surface flanked by the active site of the enzyme, respectively. The structure of I^C in complex with CPY consists of one major β-type domain and an N-terminal helical segment (Fig2). The N-terminal segment is the helical region 1 (HR1), which is formed by one 3_{10}-helix (η1) and two α-helices (α1-2) and is in direct contact with CPY. The major domain is made up of three segments: the strand-rich region 1 (SR1), strand-rich region 2 (SR2), and helical region 2 (HR2). I^C is also revealed to have the ligand-binding site, which is conserved among PEBPs and the putative binding site of the polar head group of phospholipid.

Figure 1. Ribbon drawing of the I^C-CPY complex at 2.7 Å resolution. I^C and CPY are shown in blue and green, respectively. Sulfate ions are represented by red spheres.

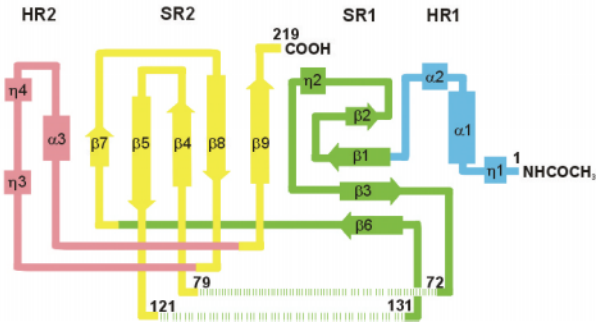


Figure 2. A topology diagram of the secondary-structure elements in I^C. β-Strands (β1-9) are represented by arrows, and α-helices (α1-3) and 3_{10}-helices (η1-4) by rectangles.

To further clarify the proteinase-inhibition mode of I^C indicated by the three-dimensional structure of the complex, we analysed the biochemical properties of various I^C mutants: the N-terminal unacetylated form (unaI^C), an N-terminal modified form with the substitution of Gly for the acetyl group (gI^C), the N-terminal seven-residues deleted form (d1-7I^C), and the unacetylated and C-terminal deleted form (d217-219I^C). The inhibition of anilidase activity of CPY by the native and mutant forms of I^C showed that the inhibitor constants, *K*i, for unaI^C, gI^C, and d217-219I^C were increased by 590-, 180-, and 550-fold, respectively, over that of the native and that the N-terminal deleted mutant (d1-7I^C) had no detectable inhibitory activities against CPY (Fig3). These results indicate that the N-terminal acetyl group has optimal properties for the efficient inactivation of CPY and that the N-terminal seven residues of I^C, designated as the N-terminal inhibitory reactive site, are absolutely essential for the inhibitory activity of I^C in solution.

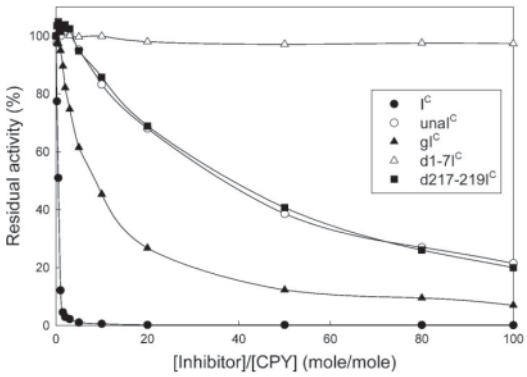


Figure 3. Stoichiometry of CPY inhibition by I^C and its mutants.

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

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

Assist Prof
TSUJI, Hayato
(D Eng)

PD
SASE, Shohei
(D Sc)

Students

SON, Eun-Choel (D3)
FUKAZAWA, Aiko (D2)
INOUE, Tomoyuki (M2)
TAKASHIMA, Yohei (M2)
KOMATSU, Shigeo (M1)

Scope of Research

Our research is concerned with some new aspects in the elemento-organic chemistry, including (1) elucidation of the σ-conjugation in the polysilanes using the configuration-constrained oligosilane model systems, (2) development of intramolecular electron transfer systems through σ-conjugated oligosilane chains, (3) construction and application of new polycyclic systems including main group elements, (4) development of new efficient reactions using main group element reagents and transition metal complex catalysts, and (5) design and synthesis of novel π-conjugated systems containing main group elements.

Research Activities (Year 2005)

Presentations

Conformation Control of Oligosilanes Based on Bicyclic Di- and Trisilane Units, Tsuji H, Fukazawa A, Tamao K, The 38th Silicon Symposium, 2 - 5 June, Boulder, USA.

All-anti Oligosilanes: Conformation Control of Oligosilanes Utilizing the Bicyclic Trisilane Unit, Fukazawa A, Tsuji H, Yamaguchi S, Tamao K, The 14th International Symposium on Organosilicon Chemistry, 31 July - 5 August, Würzburg, Germany.

Synthesis, Structure, and Photophysical Properties of Disilatriptycene Oligomers, Sase S, Tsuji H, Kawachi A, Wakamiya A, Yamaguchi S, Tamao K, The 14th International Symposium on Organosilicon Chemistry, 31 July - 5 August, Würzburg, Germany.

Grants

Tsuji H, Synthesis and Photophysical Properties of Porphyrin-Oligosilane Hybrid Molecules, Grand-in-Aid on Priority Areas, April 2004 - March 2006.

Tsuji H, Establishment of Conformation Control Method of Polysilanes Based on Bicyclic Trisilane Unit, Grand-in-Aid for Young Scientists (B), April 2005 - March 2007.

Awards

Fukazawa A, The Best Oral Presentation Award, The 85th Annual Meeting of the Chemical Society of Japan, 27 March.

Fukazawa A, Award for the First Place Poster Contribution, The 14th International Symposium on Organosilicon Chemistry, 5 August.

Fukazawa A, Student Poster Award, PACIFICHEM 2005, 18 December.

The former professor Kohei Tamao retired on 31 March 2005.

Zinc Porphyrin–fullerene Dyad Linked by σ-Conjugated Oligosilane Chains

Oligosilanes are regarded as a pseudo one-dimensional molecular wire and attract much attention due to their unique photophysical and electronic properties, as ascribed to σ-conjugation. To evaluate the electron transfer ability of the σ-conjugated Si–Si chain, we have developed various zinc porphyrin (ZnP)–fullerene(C_{60}) dyads connected by oligosilane chains, shown in Chart 1. Their photoinduced processes have been studied using the time-resolved fluorescence and absorption measurements. Photoexcitation of the dyads caused energy- and/or electron-transfer from the excited-singlet state of the ZnP to C_{60} moieties. The charge-separation takes place as the final step in the excited sate process to yield the radical-ion pair with a radical cation on the ZnP and a radical anion on the C_{60}, similar to other porphyrin–fullerene dyads. The result shows that the oligosilane chains play an important role as a good molecular wire.

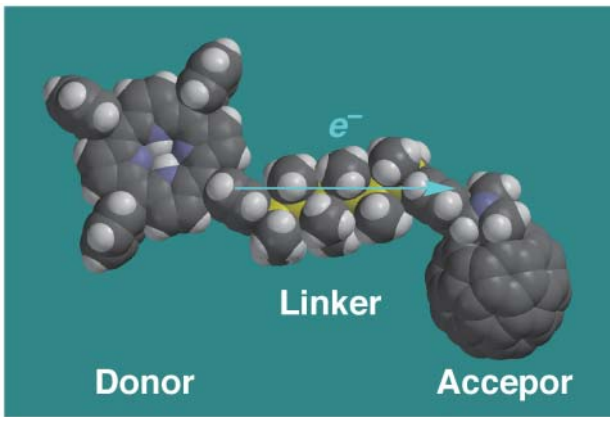


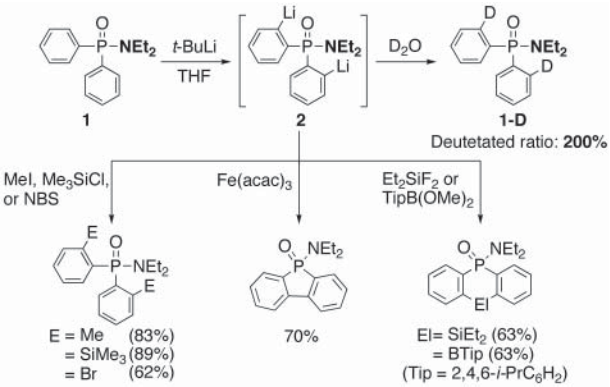
Chart 1.

Double ortho-lithiation of Aromatic Ring

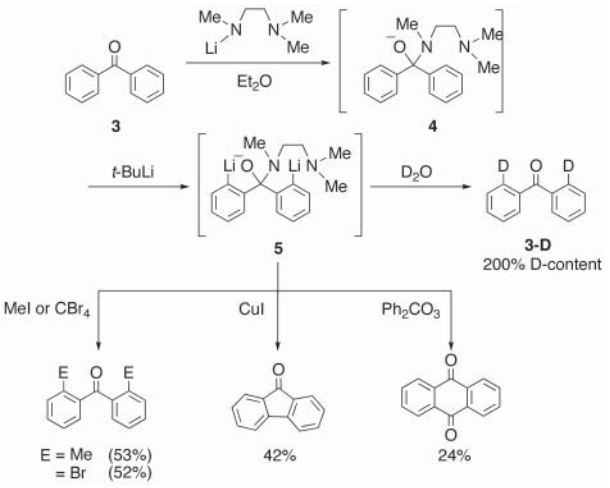
Direct metalation on the aromatic ring is a versatile method for the preparation of functionalized aromatic compounds from the viewpoint of synthetic efficiency. Most of the preceding reports are on single-metalation, by which one aromatic ring is metalated with the assistance of the directing group. In contrast, there are a few examples regarding double ortho-metalation, where two aromatic rings are metalated simultaneously by the assistance of two directing groups. We have recently developed the methods for double ortho-lithiation of a diphenylphosphorylamide and benzophenone.

Quantitative double ortho-lithiation of phosphorylamides **1** was accomplished through treatment of **1** with *tert*-butyllithium (Scheme 1). In this reaction, the amino moiety and the oxygen of the phosphoryl group are considered to act properly as directing groups, allowing the efficient double ortho-lithiation.

For double ortho-lithiation of benzophenone **3**, it is essential to introduce a trimethylethylenediamino moiety as an auxiliary directing group. Subsequent treatment of the resulting species **4** with *tert*-butyllithium afforded the double ortho-lithiated species **5** (Scheme 2). The double ortho-lithiated species **2** and **5** underwent the reaction with electrophiles, the intramolecular oxidative coupling to afford the five-membered ring compounds, and the intramolecular cyclization with the difunctional electrophiles to give the six-membered ring compounds.



Scheme 1.



Scheme 2.

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

http://msk2.kuicr.kyoto-u.ac.jp/

Prof
TAKANO, Mikio
(D Sc)

Assist Prof
SAITO, Takashi
(D Sc)

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

Students

KAN, Daisuke (D3)
YAMADA, Ikuya (D3)
HAYAMI, Arata (M3)
TAKATA, Kazuhide (M2)
TAKEDA, Yuhki (M2)
TSUJIMOTO, Yoshihiro (M2)
OKA, Kengo (M1)
HIRAI, Shigeto (M1)
HORIUCHI, Daisuke (M1)

Visitor

Prof ATTFIELD, John Paul University of Edinburg, UK, 1 July - 31 March 2005

Scope of Research

Novel inorganic materials and devices that have new, useful or exotic features such as superconductivity, ferromagnetism and quantum spin ground state are synthesized and fabricated by novel methods. For example:

- Oxides containing transition-metal ions in unusually high-valence state.
- Nonequilibrium materials that can be obtained by high pressure method or epitaxial thin film deposition method.
- Inorganic nanomaterials with useful functionality such as superparamagnetism and quantum size effect.

Research Activities (Year 2005)

Presentations

High-pressure Synthesis of a New Ferromagnetic Ferroelectric Material Bi_2NiMnO_6, Takata K, Azuma M, Saito T, Shimakawa Y, Takano M, 60th Annual Meeting, The Physical Society of Japan, 24 - 27 March (Tokyo).

Synthesis of Monodisperse, Submicron-Sized Spherical V_2O_5 Particles, Yamamoto S, Shimakawa Y, Takano M, MRS Spring Meeting 2005, 28 March - 1 April (San Francisco CA).

Synthesis of Ferromagnetic, Ferroelectric Bismuth Double-perovskite, Takata K, Azuma M, Saito T, Shimakawa Y, Takano M, 97th Sprig Meeting, The Japan Society of Powder and Powder Metallurgy, 1 - 3 June (Tokyo).

Synthesis and Magnetic Characterization of $L1_0$-FePt Nanocrystals Dispersed in Solvent, Yamamoto S, Morimoto M, Ono T, Takano M, 50th Magnetism and Magnetic Materials Conference, 30 October - 3 November (San Yose CA).

Single Crystal Growth of a Layered Cobalt Oxide $(Sr,Ba)Co_6O_{11}$ under High Pressure, and Its Magnetism, Saito T, Takeda Y, Ishiwata S, Shimakawa Y, Takano M, The 46th Annual High Pessure Conference of Japan, 31 October, Muroran Institute of Technology.

Designed New Ferroelectric, Ferromagnetic Materials -Bi_2NiMnO_6 and Bi_2CoMnO_6-, Takata K, Azuma M, Shimakawa Y, Takano M, MRS Fall Meeting 2005, 28 November - 1 December (Boston MA).

Grant

Takano M, Chemistry and Physics of 3d Transition Metal Oxides Equipped with Deep 3d Levels: Search for New Materials and New Functions, Grant-in-Aid for Scientific Research (S), 1 April 2005 - 31 March 2010.

Awards

Takano M, The L'Oreal Art & Science of Color Prizes: The 8th Gold Prize, Microstructure and Formation Process of the Characteristic Reddish Color Pattern "Hidasuki" on Bizen Stoneware: Reactions Involving Rice Straw, The L'Oreal Art & Science Foundation, 21 October 2005.

Saito T, Encouragement Prize of the Japan Society of High Pressure Science and Technology, Search of Transi-

Blue-Light Emission at Room Temperature from Ar^+-irradiated $SrTiO_3$

Oxide-based electronic devices are expected to have fascinating properties, unlike those of conventional semiconductors. Perovskite structure transition-metal oxides are key materials for this new field of electronics. Among them, $SrTiO_3$ is of particular important from the viewpoints of fundamental solid-state physics, solid-state chemistry and technological applications. We found that Ar^+-irradiated, metallic $SrTiO_3$ crystal emits 430-nm blue-light at room temperature. The oxygen-deficient metallic $SrTiO_3$ thin films grown under low-oxygen pressure also show the blue-light emission. Therefore we concluded that the Ar+-irradiation introduces oxygen deficiencies in the crystal surface, and that the deficiencies generate conduction carriers and play an important role in the emission. A model by which the doped conduction electrons and the exited holes in the in-gap state produce a new radiative process that emits blue light is proposed. It is emphasized that the emitting region could be patterned into any size and shape by the local engineering of the oxygen-deficiency in $SrTiO_3$. Shown in Fig.1 are examples of patterned blue-light emission in the form of "KYOTO". By combining conventional photolithography and Ar^+-milling (irradiation), locally oxygen-deficient regions in positive and negative manners are fabricated on the stoichiometric $SrTiO_3$ substrates. In the upper panel of the figure, only the irradiated KYOTO shines in blue, whereas in the bottom panel, the non-irradiated KYOTO remains dark. This is a clear demonstration of simple method for the room-temperature blue-luminescence on macroscopic and microscopic scales. These new features of $SrTiO_3$ will open up new possibilities for the oxide-base electronic devices.

Figure 1. An example of the blue-light emission from a local engineered region of oxygen vacancies in $SrTiO_3$.

Size-Controlled Synthesis of Monodisperse Spherical V_2O_5 Particles

We developed a method to synthesize monodisperse spherical V_2O_5 particles with various sizes via hydrolysis of vanadium isopropoxide in acetone/pyridine mixture solution under air. In Fig.2, their average size (D) and the standard deviation (σ) are plotted against the concentration of pyridine (C). Fig.3 clearly shows that the size and its distribution are strongly dependent on C. At low C ($C < 2.5$ wt%), they are small and rather polydisperse. However, at higher C ($C > 2.5$ wt%), the situation drastically changes. They become monodisperse, their size distribution being as low as ca. 7%. It is worthwhile to note that the size of them can be controlled from about 200 to 800 nm by changing the concentration of pyridine while keeping their narrow size distribution. Such monodisperse V_2O_5 particles are possibly used in catalysis, lithium ion battery, electrochromic device, sensors and actuators.

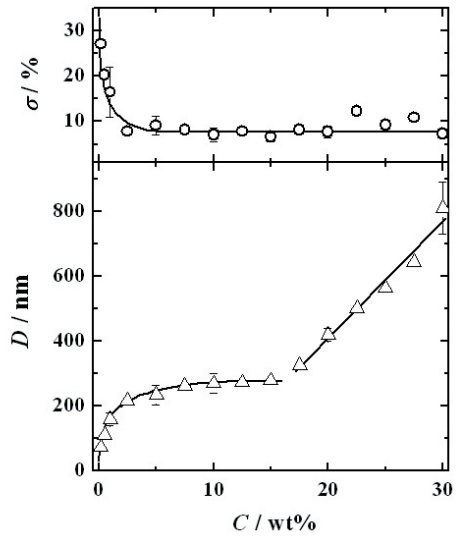


Figure 2. Plots of D (open triangles) and σ (open circles) as a function of C. Solid lines are guide to eyes.

tion Metal Oxides and Development of Single Crystal Growth Technique Using High Pressure Method, The Japan Society of High Pressure Science and Technology, 30 October 2005.

International Research Center for Elements Science - Organotransition Metal Chemistry -

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

Prof
OZAWA, Fumiyuki
(D Eng)

Assoc Prof
OKAZAKI, Masaaki
(D Sc)

Assist Prof
KATAYAMA, Hiroyuki
(D Eng)

PD
MUTOH, Yuichiro
(D Eng)

Students

NAGAO, Masato (D3)
MURAKAMI, Hiromi (D2)
WAKIOKA, Masayuki (D2)
JENSEN, Rader S (D2)
HAYASHI, Akito (D1)
WATANABE, Emiko (M2)
HAYASHI, Kyohei (M1)
YOSHITOMI, Takahiko (M1)
YOSHIMURA, Ken-ichi (M1)
UEHIRA, Kousei (UG)
YAMAMOTO, Yasutaka (UG)

Scope of Research

This laboratory aims at establishment of new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using kinetic techniques on the reaction intermediates and elementary processes. The research subjects include: (1) development of novel ligand systems for catalysis, (2) functionalization of organic substrates on transition-metal clusters, and (3) development of highly efficient ways of constructing functional organic molecules.

Research Activities (Year 2005)

Presentations

Stereocontrolled Synthesis of All-cis Poly(phenylene vinylene)s (PPVs): A Novel Method For Direct Micropatterning of PPVs, Ozawa F, The 4th International Symposium of the Kyoto COE Project "Elements Science", 6 - 7 January, Kyoto, Japan.

(*Z*)-Selective Cross-Dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinylideneruthenium Complexes, Katayama H, Ozawa F, The 4th International Symposium of the Kyoto COE Project "Elements Science", 6 - 7 January, Kyoto, Japan.

Stereocontrolled Synthesis and Optical Properties of All-cis Poly(phenylene vinylene)s (PPVs): A Novel Method for Direct Patterning of PPVs, Katayama H, Nagao M, Nishimura T, Matsui Y, Umeda K, Akamatsu K, Tsuruoka T, Nawafune H, Ozawa F, The 8th SPSJ International Polymer Conference (IPC2005), 26 - 29 July, Fukuoka, Japan.

Stereocontrolled Synthesis and Optical Properties of All-cis Poly(phenylene vinylene)s (PPVs): An Extremely Simple Method for Direct Patterning of PPVs, Katayama H, Ozawa F, The 4th Asian-European Symposium, 6 - 9 November, Nagasaki, Japan.

Highly (*Z*)-Selective Hydrosilylation of Terminal Alkynes Catalyzed by Diphosphinidenecyclobutene Ruthenium Complex: Application to the Synthesis of (*Z*,*Z*)-Bis(2-bromoethenyl)arenes, Katayama H, Ozawa F, The 13th Korea-Japan Joint Symposium on Organometallic and Coordination Chemistry, 23 - 26 November, Jeju, Korea.

Stepwise Halogenation of Acetylene on the Tetrairon Core: Systematic Synthesis and Property of Haloacetylene-Coordinated Clusters, Okazaki M, Takano M, Yoshimura K, Tobita H, Ozawa, F, Singapore International Chemical Conference 4 (SICC-4), 8 - 10 December, The Shangri-La, Singapore.

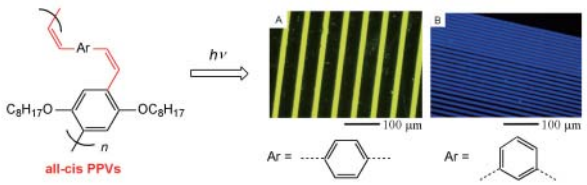
An Ethynyl Cation on the Butterfly-type Tetrairon Core, Okazaki M, Takano M, Yoshimura K, Tobita H, Ozawa, F, PACIFICHEM2005, 15 - 20 December, Honolulu, Hawaii, USA.

Alkyne-insertion into *cis*-Pt(ER_3)($SnMe_3$)L_2 Complexes (E = Si, Ge), Ozawa, F, PACIFICHEM2005, 15 - 20 December, Honolulu, Hawaii, USA.

Highly Active Catalysts Bearing Diphosphinidenecyclobutene Ligands, Ozawa, F, The 6th Journal of Organometallic Chemistry Symposium, 17 - 18 December, Honolulu, Hawaii, USA.

Stereocontrolled Synthesis and Optical Properties of All-cis Poly(phenylene vinylenes) (PPVs): A Method for Direct Patterning of PPVs

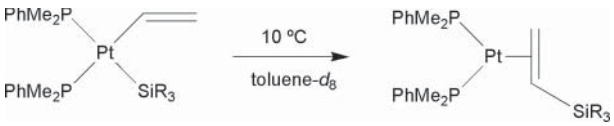
Poly(phenylene vinylenes) (PPVs) belong to the group of π-conjugated polymers that have applications in light-emitting diodes (LEDs), lasers, and solar cells. Although stereoregularity of vinylene linkages in the polymer backbone is also known to profoundly affect the optical properties of PPVs, efficient ways of regulating the geometries of vinylene linkages have remained almost unexplored. Geometrically pure, all-cis poly(phenylene vinylenes) (PPVs) are synthesized by Suzuki-Miyaura-type polycondensation of 2,5-dioctyloxy-1,4-benzenediboronic acid with (*Z*,*Z*)-bis(2-bromoethenyl)benzenes, which are prepared by ruthenium-catalyzed (*Z*)-selective double hydrosilylation of diethynylbenzenes, followed by bromodesilylation of the resulting (*Z*,*Z*)-bis(2-silylethenyl)benzenes with *N*-bromosuccinimide. The all-cis PPVs thus obtained undergo one-way photoisomerization to the corresponding *trans*-PPVs both in solution and in the solid. This phenomenon is applied to direct microscale patterning of PPVs onto a quartz substrate.



Scheme 1. Fluorescent images of micropatterned all-cis PPVs.

C-Si Reductive Elimination from *cis*-Vinyl(silyl)platinum(II) Complexes

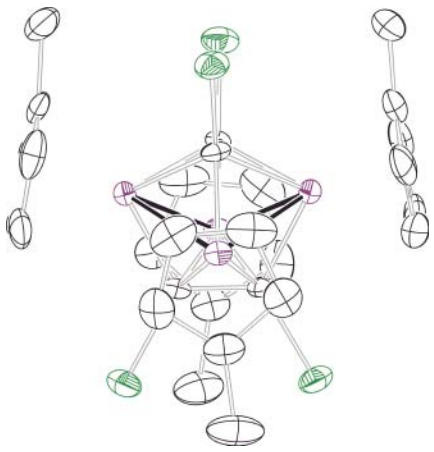
While the transition-metal-catalyzed silylation reactions of unsaturated hydrocarbons such as hydrosilylation, bis-silylation, and borylsilylation are generally assumed to involve C-Si reductive elimination as the product-forming step, detailed information on this elementary process has been limited. The complexes *cis*-$Pt(CH{=}CH_2)(SiR_3)(PMe_2Ph)_2$ (R_3=Ph_3, $(C_6H_4Me\text{-}p)_3$, $MePh_2$, FPh_2) have been prepared by the reactions of *trans*-$PtCl(SiR_3)(PMe_2Ph)_2$ with $Mg(CH{=}CH_2)_2$ in THF, followed by *trans-cis* isomerization of the resulting *trans*-alkenyl(silyl) complexes in solution promoted by CO. The Complexes undergo C-Si reductive elimination in toluene-d_8 to give platinum(0) complexes coordinated with vinylsilanes. Kinetic data have suggested a direct reaction path without dissociation of the phosphine ligand.



Scheme 2. C-Si Reductive elimination from Pt(II) complexes.

Synthesis and Property of BrCCH- and BrCCBr-Coordinated Tetrairon Clusters

Haloalkynes have been recognized as useful C_2 synthetic intermediates in organic chemistry. However, the coordination chemistry of haloalkyenes has yet to be explored in detail. We succeeded in the stepwise bromination of two acetylene ligands in $[(\eta^5\text{-}C_5H_4Me)_4Fe_4(HCCH)_2]^+$ using *N*-bromosuccinimide (NBS). The bromoacetylene part displays high reactivities toward a variety of nucleophiles such as water, ZnR_2 (R=Me, Et), HC≡CMgBr, Li*p*Tol, pyridine, and 4,4'-bipyridyl.



Scheme 3. Molecular structure of $[(\eta^5\text{-}C_5H_4Me)_4Fe_4(BrCCBr)_2]^+$.

Grants

Ozawa F, Reaction Control of Catalytic Intermediates, Grant-in-Aid for Scientific Research on Priority Areas, October 2002 - March 2006.

Ozawa F, Novel Organometallic Complexes with Phophaalkene Ligands: Synthesis and Catalysis, Grant-in-Aid for Scientific Research (B) (2), April 2003 - March 2006.

Okazaki M, Chemistry of "Ethynyl Cation"-Coordinated Transition-Metal Clusters, Grants-in-Aid for Young Scientists (B), April 2005 - March 2007.

International Research Center for Elements Science - Photonic Elements Science -

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

Prof
KANEMITSU, Yoshihiko
(D Eng)

Assoc Prof
MATSUDA, Kazunari
(D Eng)

Assist Prof
INOUYE, Hideyuki
(D Eng)

Res
HIRORI, Hideki

Students

HIRANO, Daisuke (M1)
INOUE, Tadashi (M1)
ITO, Yuichi (M1)

Scope of Research

Our research interest is to understand optical and quantum properties of nanostructures and nanomaterials and to develop 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 scanning near-field optical microscope, (2) Development of nanoparticle assembly with new optical functionalities, and (3) Ultrafast optical spectroscopy of excited states of semiconductor nanostructures.

Research Activities (Year 2005)

Presentations

Luminescence of Impurity-Doped Semiconductor Nanoparticles (invited), Kanemitsu Y, International Conference on Dynamical Processes in Excited State of Solids, DPC, 1 - 5 August 2005, Shanghai, China.

Direct Observation of Exciton Wavefunction in a Semiconductor Quantum Dot by Near-Field Scanning Optical Microscope (invited), Matsuda K, Annual Meeting of Physical Society of Japan, 24 - 27 March 2005, Chiba, Japan.

Luminescence Properties of Semiconductor Nanoparticles (invited), Kanemitsu Y, The 65th Autumn Meeting of The Japan Society of Applied Physics, 29 March - 1 April 2005, Saitama, Japan.

Light-Emitting Nanoparticles (invited), Kanemitsu Y, The 65th Autumn Meeting of The Japan Society of Applied Physics, 29 March-1 April 2005, Saitama, Japan.

Grants

Kanemitsu Y, Basic Research for Development of Near-Field Optical Microscope for Elemental Analysis and Mass Spectrometry, Grant-in-Aid for Exploratory Research, 1 April 2005 - 31 March 2007.

Matsuda K, Explorer of Optical Properties and Application of Quantum Optical Devices in an Individual Carbon-Nanotube by Optical Nanoprobing, Grant-in-Aid for Young Scientists (A), 1 April 2005 - 31 March 2008.

Matsuda K, Wavefunction Imaging and Control in Semiconductor Nano-structure by Ultimate Optical Nanoprobe, Precursory Research for Embryonic Science and Technology, Japan Science and Technology Agency, 1 November 2002 - 31 March 2006.

Matsuda K, Development of Near-Field Scanning Optical Microscope with Nanometer-Level Spatial Resolution, Research Foundation for Opto-Science and Technology, Research Grant, 1 April 2005 - 31 March 2006.

Matsuda K, Explorer of Properties and Application of Quantum Devices in Carbon-Nanotubes by Optical Nanoprobing, Foundation for C&C Promotion, Research Grant for Young Scientists, 1 April 2005 - 31 March 2006.

Inouye H, Luminescence Dynamics of Self-Assemble Nanocrystal Composite Film and Study for Realizing High Luminescence Efficiency, Grant-in-Aid for Young Scientists (B), 1 April 2005 - 31 March 2007.

Award

Kanemitsu Y, The Ichimura Prize, Pioneering Contributions for Light Emitting Nanoparticles, 28 April 2005.

An Individual Single-Walled Carbon Nanotube Spectroscopy

Single-walled carbon nanotubes have attracted a great deal of attention because of their potential use in electronic devices and their unique physical properties. We investigated photoluminescence properties of individual micelle-encapsulated single-walled carbon nanotubes. Figure 1 shows 3-dimensional plot of a single-walled carbon nanotube photoluminescence image, detected at a range of 1.18 - 1.37 eV at room temperature. Each sharp peak corresponds to the photoluminescence signal from an individual single-walled carbon nanotube. We observed that single photoluminescence peak from isolated individual single-walled carbon nanotube showed a linear increase and saturation behavior of the photoluminescence intensity with an increase of excitation power. We also found unusual photoluminescence intensity fluctuation in the temporal evolutions of the photoluminescence intensity, referred to as photoluminescence intermittency. The photoluminescence intensity fluctuation was seen with some single-walled carbon nanotubes, while the photoluminescence intensity with most single-walled carbon nanotubes remained at a constant amplitude. The photoluminescence intermittency is attributed to the fluctuation of induced local electric field by trapped charges around single-walled carbon nanotubes.

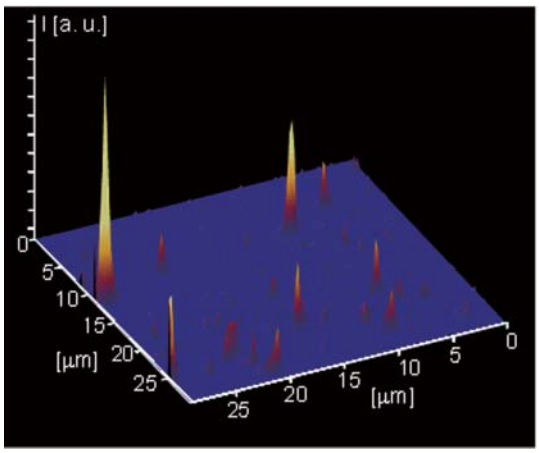


Figure 1. 3-dimensional plot of a single-walled carbon nanotube photoluminescence image by scanning confocal microscopy.

Femtosecond Laser Spectroscopy of Wide Band-Gap Semiconductors

Over the past decade, there have been many experimental and theoretical studies on the optical properties of nitride semiconductors such as GaN, $In_xGa_{1-x}N$, and $Al_yGa_{1-y}N$ crystals. In $In_xGa_{1-x}N$ ternary alloys, efficient photoluminescence (PL) is due to the exciton localization at potential minima. We have clarified the exciton localization processes in $In_xGa_{1-x}N$ ternary alloys by means of optical Kerr-gate time-resolved PL measurements. Figure 2 shows the temporal change of the PL spectra after the femtosecond laser excitation. It is clearly shown that the photogenerated carriers relax to the lower energy state within the 15 ps. Time-resolved PL spectral measurements are one of the most useful methods for understanding the exciton localization dynamics and the radiative recombination processes in semiconductor mixed crystals.

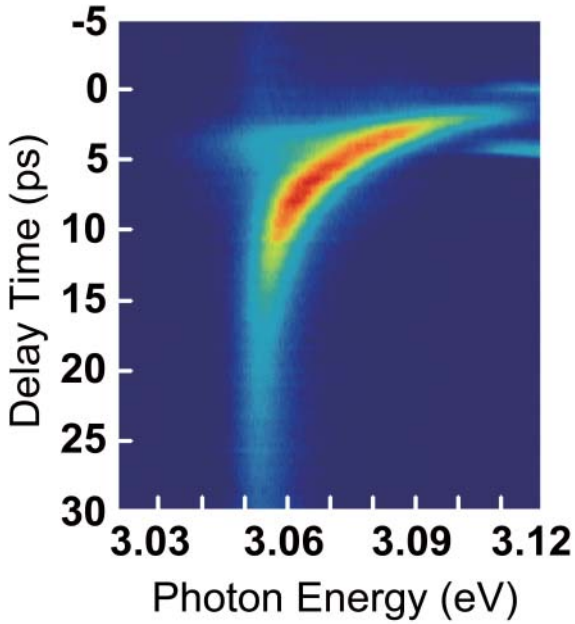


Figure 2. Time-resolved PL spectra of the $In_xGa_{1-x}N$ thin film.

Bioinformatics Center
- Bioknowledge Systems -

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

Prof
KANEHISA, Minoru
(D Sc)

Assoc Prof
GOTO, Susumu
(D Eng)

Assist Prof
HATTORI, Masahiro
(D Sc)

Vis Assist Prof
AOKI-KINOSHITA, Kiyoko
(Ph D)

Vis Assit Prof
ITOH, Masumi

PD
KAWANO, Shin
(D Eng)

PD
SCHWARTZ, Jean-Marc
(D Eng)

PD
TANAKA, Nobuya
(D Eng)

PD
OKAMOTO, Shinobu
(D Sc)

PD (JSPS)
KARLSSON-WHEELOCK, Åsa
(Ph D)

PD (JSPS)
WHEELOCK, Craig
(Ph D)

PD
KADOWAKI, Tadashi
(D Sc)

PD
MASOUDI-NEJAD, Ali
(Ph D)

PD
HUANG, Jian
(Ph D)

PD
HAYES, Nelson
(Ph D)

PD (JSPS)
GUTTERIDGE, Alexander
(Ph D)

Research Associates (pt)

LIMVIPHUVADH, Vachiranee
HIZUKURI, Yoshiyuki

Researcher

HIRAKAWA, Mika

Students

MINOWA, Yosuke (D3)
YAMADA, Takuji (D3)
OKUDA, Shujiro (D3)
MORIYA, Yuki (D3)
FUJITA, Masashi (D3)
SAKIYAMA, Tadahiko (D2)
TANAKA, Michihiro (D2)
SAKAI, Hiroki (D2)
OH, Min-A (D2)
ONUKI, Ritsuko (D1)
SHIGEMIZU, Daichi (D1)
HONDA, Wataru (M2)
HASHIMOTO, Kosuke (M2)
MUTO, Ai (M2)
SAITO, Koichi (M2)
TSUCHIDA, Akira (M1)
TAKARABE, Masataka (M1)
HAMADA, Yusuke (M1)
YOSHIZAWA, Akiyasu (RF)

Scope of Research

Owing to continuous developments of high throughput experimental technologies, projects are going on not only to determine complete genome sequences of an increasing number of organisms, but also to analyze gene expression profiles both at the mRNA and protein levels and to catalog protein 3D structure families. Bioinformatics provides basic concepts as well as practical methods to go up from the molecular level to the cellular level, and eventually to still higher levels, to that of biological systems by analyzing complex interactions among building blocks and with dynamic environments. We have been developing such bioinformatics technologies and the KEGG system (http://www.genome.jp/kegg/), which is our attempt to uncover and utilize cellular functions through the reconstruction of protein interaction networks from genome information.

Research Activities (Year 2005)

Grants

Kanehisa M, Education and Research Organization for Genome Information Science, MEXT.

Kanehisa M, BRITE: Deductive Database of the Genome and the Biological System Based on Binary Relations, Bioinformatics Research and Development, JST.

RPAIR: a Database of Chemical Transformation Patterns in Enzymatic Reactions

Chemical genomics is the next stage of post-genomic analysis. Drugs, environmental substances and various chemical compounds contribute to the fluctuation of bio-systems. Therefore, chemical genomic analysis would require the investigation of relationships between genomes and their extracellular environments.

These relationships between bio-systems and environments include complicated biochemical reactions. At present, biochemical reactions are hierarchically classified using EC (Enzyme Commission) numbers. However, the classification is not totally based on chemical reactions, but also include enzymes or enzyme genes. EC numbers are commonly utilized as identifiers of enzymes or enzyme genes.

In order to expand our current limited knowledge on biochemical reactions as represented by EC numbers, we developed a novel database that provides the patterns of the conformational changes between the chemical structures of the substrate and product. This database is integrated into the KEGG resource, so other databases in KEGG have links to the entries of this database. All of the data is available from http://www.genome.jp/reaction/.

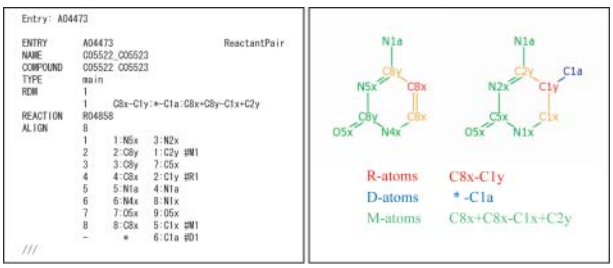


Figure 1. An RPAIR database entry (left) and the assignment of R-, D- and M- atoms (right).

KAAS : an Automatic Functional Annotation Server for New Genomes

KEGG Orthology (KO), which is developed from the "Ortholog ID", an extension of the EC number in the KEGG PATHWAY database, is one of our major projects and is intended to identify and classify orthologous gene clusters among all species computationally and manually.

Recently, a number of draft- and completely - sequenced genomes are rapidly growing. Therefore, we need a speedy and easy method to annotate gene functions. KEGG Automatic Annotation Server (KAAS), which is a web-based server, provides functional annotation of genes by BLAST comparisons against the manually curated KEGG GENES database and a heuristic method. The result contains hierarchical KO assignments and automatically generated KEGG pathways. We have been using this method effectively to annotate draft genomes and EST clusters, which we provide as the DGENES and EGENES databases.

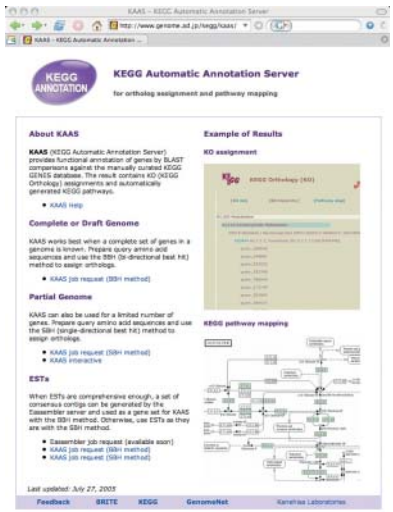


Figure 2. KAAS: KEGG Automatic Annotation Server (http://www.genome.jp/kegg/kaas/).

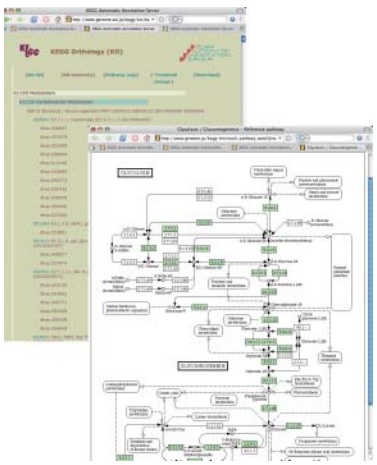


Figure 3. Results of KAAS. KO assignment (left) and generated pathway (right).

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

Kanehisa M, Biological Systems Database, Grants-in-Aid for Scientific Research on Priority Areas, MEXT.

Kanehisa M, Bioinformatics Training Unit; Education and Research Organization for Genome Information Science. MEXT.

Goto S, Probing the *Plasmodium falciparum* Genome, Contact Research, JST.

Bioinformatics Center
- Biological Information Networks -

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

Prof
AKUTSU, Tatsuya
(D Eng)

Assist Prof
UEDA, Nobuhisa
(D Eng)

Assist Prof
HAYASHIDA, Morihiro
(D Inf)

Guest Res Assoc
NACHER, Jose C.
(Ph D)

PD
MATSUDA, Setsuro
(D Eng)

PD
OCHIAI, Tomoshiro
(D Sc)

Students

FUKAGAWA, Daiji (D3)
K. C., Dukka Bahadur (D3)
SAIGO, Hiroto (D3)
TAMADA, Yoshinori (D3)
MEIRELES, Lidio (M2)
BROWN, John (M1)
OOTAKA, Ryu (M1)
SAKAI, Daisuke (M1)
TAKEUCHI, Shigeki (M1)
POOLSAP, Unyanee (RS)

Visitors

Prof ZHANG, Xiang-Sun	Chinese Academy of Sciences, 16 May 2005
Dr VERT, Jean-Philippe	Ecole des Mines de Paris, France, 11 - 21 October 2005
Dr YAMANISHI, Yoshihiro	Ecole des Mines de Paris, France, 31 October - 2 November 2005
Mr MAHÉ, Pierre	Ecole des Mines de Paris, France, 5 - 17 December 2005

Scope of Research

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

Research Activities (Year 2005)

Presentations

Clique Based Algorithms for Protein Threading with Profiles and Constraints, K.C. D, Tomita E, Suzuki J, Horimoto K, Akutsu T, The 3rd Asia-Pacific Bioinformatics Conference, 18 January.

On Construction and Transformation of Scale-free Networks, Akutsu T, The 50th NIBB Conference on Structure and Dynamics of Complex Biological Networks, 8 February.

Inferring a Graph from Path Frequency, Akutsu T, Fukagawa D, The 16th Annual Symposium on Combinatorial Pattern Matching, 22 June.

On Transformation and Construction of Scale-free Networks, Akutsu T, International Workshop on Complex Networks, 24 June.

Kernel-based Approaches to Classification and Design of Protein Sequences and Chemical Compounds, Akutsu T, 2005 International Joint Conference of InCoB, AASBi, and KSBi, 22 September.

On Structures of Metabolic Networks and Protein-Domain Networks, Akutsu T, Mathematical Analysis of Complex Phenomena in Life Sciences, 26 October.

Grants

Akutsu T, Miyano S, Maruyama O, Ueda N, Algorithms for Extracting Common Patterns from Structured Biological Data, Grant-in-Aid for Scientific Research (B), 1 April 2004 - 31 March 2008.

Akutsu T, Mathematical Analysis of Structure and Dynamics of Biological Information Networks, Grant-in-Aid

A Novel Representation of Protein Sequences for Prediction of Subcellular Location Using Support Vector Machines

As the number of complete genomes increases, accurate methods to automatically predict subcellular locations of proteins are increasingly helpful to annotate their biological functions. In order to improve predictive accuracy of the many prediction methods developed to date, we have proposed a novel representation of protein sequences. This representation involves local compositions of amino acids and twin amino acids, and local frequencies of distance between successive (basic, hydrophobic, and other) amino acids. For calculating the local features, each sequence is split into the N-terminal, middle, and C-terminal parts. The N-terminal part is further divided into four regions to consider ambiguity in the length and position of signal sequences. We tested this representation with support vector machines on two data sets extracted from the SWISS-PROT database. Despite simplicity of the representation, overall accuracies of our method were more than 87% and 91% for eukaryotic and prokaryotic proteins, respectively. These are almost the highest accuracy among the methods using sequence information alone. Based on the above methodology, we have also developed a web server, SLP-Local (http://mint.kuicr.kyoto-u.ac.jp/~smatsuda/slplocal.html).

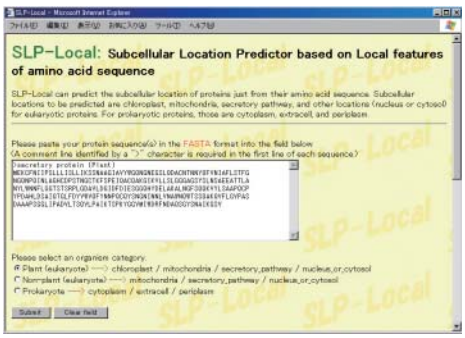


Figure 1. A snapshot of the top page of SLP-Local.

Matsuda, S., Vert, J.-P., Saigo, H., Ueda, N., Toh, H., and Akutsu, T. (2005) *Protein Sci.*, **14**, 2804-2813.

Protein Domain Networks: Scale-Free Mixing of Positive and Negative Exponents

Proteins are essential molecules and responsible for most cellular processes. A protein region with well-defined structural and functional properties is called *protein domain*.

Here, we present a theoretical model for studying the protein domain networks, where one node of the network corresponds to one protein and two proteins are connected if they contain the same domain. The resulting distribution of nodes with a given degree, k, shows not only a power-law with negative exponent $\gamma = -1$, but it resembles the superposition of two power-law functions, one with a negative exponent and another with a positive exponent $\beta = 1$. We call this distribution pattern "*scale-free mixing*". To explain the emergence of this superposition of power-laws, we propose a basic model with two main components: (1) mutation and (2) duplication of domains. Precisely, duplication gives rise to complete subgraphs (i.e., cliques) on the network, thus for several values of k a large number of nodes with degree k is produced, which explains the positive power-law branch of the degree distribution.

The results of our model were compared with protein domain networks of six organisms generated with data from the Uniprot Knowledgebase-Swissprot database for protein sequences and using InterPro, Pfam and Smart for domain databases. Our results indicate that the signal of this positive power-law branch of the measured distribution is observed in experimental data and it is conserved among organisms from *E. coli* to *H. sapiens*.

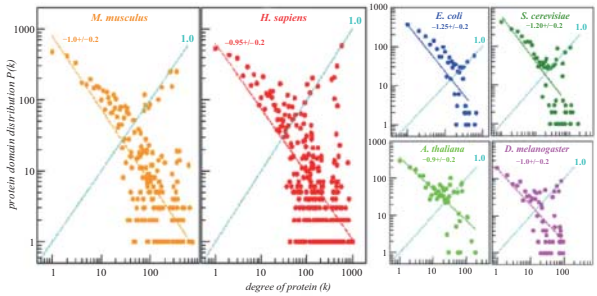


Figure 2. The degree distribution $P(k)$ of the protein domain network in *M. musculus, H. sapiens, E. coli, S. cerevisiae, A. thaliana and D. melanogaster* organisms exhibits a *scale-free mixing* pattern.

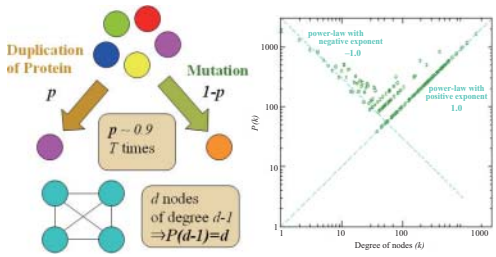


Figure 3. Scheme of the process that generates a *scale-free mixing* distribution, and the results of our proposed model.

Nacher J. C., Hayashida M., Akutsu, T., Protein domain networks: scale-free mixing of positive and negative exponents, *Physica A*, in press.

for Priority Area Research, 1 April 2005 - 31 March 2010.

Ueda N, Statistical Language Models that Generate a Pair of Sequences for Sequence Analysis, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2003 - 31 March 2006.

Bioinformatics Center
- Pathway Engineering -

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

Prof
MAMITSUKA, Hiroshi
(D Sc)

Assist Prof
TAKIGAWA, Ichigaku
(D Eng)

PD
WAN, Raymond
(Ph D)

PD
ZHU, Shanfeng
(Ph D)

Scope of Research

With the recent advance of experimental techniques in molecular biology and biochemistry, the research in modern life science is shifting to the comprehensive understanding of a biological mechanism carried out by a variety of biological molecules, including genes, proteins and chemical compounds. The focus of our laboratory is placed on such molecular mechanisms in biological phenomena, represented by biological networks such as gene regulatory networks, metabolic pathways and signal transduction pathways. They are graphs, trees and/or networks in a general computer science terminology. The research objective of our laboratory is to develop computational techniques in computer science and/or statistics to systematically analyze and understand the principles of such biological networks at the cellular and organism level.

Research Activities (Year 2005)

Presentations

Cleaning Microarray Expression Data Using Markov Random Field Based-on Profile Similarity, Wan R, Mamitsuka H and Aoki K F, Twentieth ACM Symposium on Applied Computing, Santa Fe, NM, USA, 14 March.

Efficiently Finding Glycan Motifs Using a Profile Probabilistic Sibling-Dependent Tree Markov Model, Aoki-Kinoshita K F, Ueda N, Mamitsuka H and Kanehisa M, 25th Annual Meeting of the Japanese Society of Carbohydrate Research, Otsu, Japan, 9 July.

Analyzing Metabolic Pathways with Microarray Data Based on Mixtures of Markov Chains, Mamitsuka H, 2005 Japanese Joint Statistical Meeting, Hiroshima, Japan, 13 September.

A Probabilistic Model for Mining Implicit "Chemical Compound - Gene" Relations from Literature, Zhu S, Okuno Y, Tsujimoto G and Mamitsuka H, Fourth European Conference on Computational Biology, Mardid, Spain, 1 October.

A Tree-based Markov Model for Tree-Structure Profiles, Aoki-Kinoshita K F, Ueda N, Mamitsuka H, Goto S and Kanehisa M, Second SIGBIO Meeting, Information Processing Society of Japan, Kyoto, Japan, 7 October.

A Probabilistic Model for Mining Implicit "Chemical Compound - Gene" Relations from Literature, Zhu S, Okuno Y, Tsujimoto G and Mamitsuka H, Second SIGBIO Meeting, Information Processing Society of Japan, Kyoto, Japan, 7 October.

A Profile HMM for Tree Structures to Locate Glycan Structure Profiles, Aoki-Kinoshita K F, Ueda N, Mamitsuka H, Goto S and Kanehisa M, Annual Conference of the Society for Glycobiology, Boston, USA, 10 November.

Grant

Mamitsuka H, Probabilistic Model-based Method for Mining from Structured Data in Bioinformatics, Research Grant from Okawa Foundation for Information and Telecommunications, 1 September 2005 - 30 August 2006.

Mining Biomedical Co-occurrence Data with a Probabilistic Model

Mining literature for biomedical knowledge discovery has become a very active field in bioinformatics recently. One of the important applications is to discover the relationship among genes, proteins, disease phenotype and chemical compounds. Co-occurrence in MEDLINE is a simple and popular technique for discovering possible biological relationships among different entities. This technique is based on the following hypothesis: if biological entity A co-occurs with biological entity B in the same MEDLINE record, A and B should be biologically related with high probability. Here we also employ co-occurrence technique to identify biologically related genes and chemical compounds. We focus on discovering implicit related entities, e.g. "chemical compound - gene", being those which are not in existing co-occurrences in the literature but could be discovered from the co-occurrence data.

We made use of a probabilistic model, which we call a mixture aspect model (MAM), coupled with an efficient algorithm for estimating its parameters. MAM is an extension of a probabilistic model, called the aspect model (AM) developed in natural language processing, with one significant difference of the ability of incorporating different types of co-occurrence data efficiently. A MAM is called *k*MAM when we use *k* different types of co-occurrence data, and 1MAM is equal to AM.

We evaluated our approach by performing experiments on three types of co-occurrence data: gene-gene (GG), compound-compound (CC) and compound-gene (CG) from the MEDLINE records. We extract these data from RefSeq database and corresponding MEDLINE records. In our dataset, we have 22,292 genes and 3,454 chemical compounds. There are altogether 174,077 GG pairs, 20,443 CC pairs and 47,217 CG pairs occurring in 63940 MEDLINE documents.

We evaluated the performance of four different types of MAMs, i.e. AM, 2MAM (+CC), 2MAM (+GG) and 3MAM, using cross-validation on predicting CG pairs. AM uses CG only in training while 2MAM (+CC) uses both CG and CC, and 2MAM~(+GG) uses both CG and GG. 3MAM uses all CG, CC and GG. To examine the effect of the size of the training data set to the performance of the probabilistic model, we set five different ratios of the size of training to test data, 3:1, 2:1, 1:1, 1:2 and 1:3, in the cross-validation experiment. We carried out 50 rounds of this cross-validation to reduce possible biases occurring in only a few rounds and averaged the results obtained. When we add another type of training data, keeping the same training CG pairs for each round of cross-validation, we added one or more other types of co-occurrence data to train 2MAM (+CC), 2MAM (+GG) or 3MAM. Then, the prediction was performed on the same test dataset. We note that AM cannot make any predictions on a CG pair in the test data if one component of this pair does not appear in the training data. Thus, we removed all such co-occurrence pairs in the test data, and the remaining pairs were used as positive test examples. We then randomly generated the same number of CG pairs which are not found in both training and test as negative test examples.

Once we estimated the probability parameters of a probabilistic model from training data, we computed the likelihood of each CG pair in test data and ranked all pairs according to their likelihoods. We evaluated these ranked pairs in AUC (Area Under the ROC curve). Please note that the larger the AUC, the better the performance of the model. We further used the paired sample two-tailed *t*-test to statistically evaluate the performance difference of the two models. Table 1 shows the results.

We also computed the likelihoods of all unknown CG (more specifically, drug-gene) pairs using our approach and selected the top 20 pairs according to the likelihoods. Table 2 shows the 20 pairs. We validated them from biological, medical and pharmaceutical viewpoints.

Model	Ratio of training to test data				
	3:1	2:1	1:1	1:2	1:3
3MAM	**96.0**	**95.5**	**94.5**	**92.8**	**91.5**
2MAM (+CC)	95.0 (**81.4**)	94.5 (**73.9**)	93.2 (**60.3**)	91.1 (**88.6**)	89.6 (**94.9**)
2MAM (+GG)	92.3 (**193.8**)	91.6 (**168.0**)	89.8 (**158.6**)	87.7 (**209.2**)	86.4 (**197.4**)
AM	89.0 (**232.2**)	88.0 (**202.4**)	86.0 (**190.5**)	83.6 (**285.5**)	82.0 (**357.4**)

Table 1. Percentage of the AUCs and the *t*-values (in parentheses) obtained by 50 rounds of cross-validation on compound-gene pairs.

CAS registry number	Drug name	Locus ID	Gene name	Log-likelihood
19545-26-7	Wortmannin	5594	*MAPK1*: Mitogen-activated protein kinase 1	−2.615
16561-29-8	Tetradecanoylphorbol acetate	5590	*PRKCZ*: Protein kinase C, zeta	−2.764
23214-92-8	Doxorubicin	1029	*CDKN2A*: Cyclin-dependent kinase inhibitor 2A	−2.992
73-22-3	Tryptophan	5705	*PSMC5*: Proteasome 26S subunit	−3.000
10102-43-9	Nitric Oxide	959	*TNFSF5*: Tumor necrosis factor, member 5	−3.027
66-81-9	Cycloheximide	5970	*RELA*: V-rel reticuloendotheliosis viral oncogene homolog A	−3.030
33419-42-0	Etoposide	4193	*MDM2*: Transformed 3T3 cell double minute 2	−3.033
50-02-2	Dexamethasone	3458	*IFNG*: Interferon, gamma	−3.037
15663-27-1	Cisplatin	581	*BAX*: BCL2-associated X protein	−3.060
521-18-6	Dihydrotestosterone	2099	*ESR1*: Estrogen receptor 1	−3.061
53-85-0	Dichlororibofuranosylbenzimidazole	2963	*GTF2F2*: General transcription factor IIF, polypeptide 2	−3.103
50-07-7	Mitomycin	7157	*TP53*: Tumor protein p53	−3.104
320-67-2	Azacitidine	6622	*SNCA*: Synuclein, alpha	−3.111
33069-62-4	Paclitaxel	581	*BAX*: BCL2-associated X protein	−3.148
133407-82-6	Leucine aldehyde	7124	*TNF*: Tumor necrosis factor, member 2	−3.203
10540-29-1	Tamoxifen	5241	*PGR*: Progesterone receptor	−3.208
7722-84-1	Hydrogen peroxide	596	*BCL2*: B-cell CLL/lymphoma 2	−3.213
67526-95-8	Thapsagargin	5580	*PRKCD*: Protein kinase C, delta	−3.215
59-14-3	Bromodeoxyuridine	1027	*CDKN1B*: Cyclin-dependent kinase inhibitor 1B	−3.221

Table 2. Top 20 pairs of drugs and genes.

Bioinformatics Center
- Bioinformatics Training Unit -

http://www.bic.kyoto-u.ac.jp/toh/index_J.html

Vis Assoc Prof
KUMA, Kei-ichi
(D Sc)

Vis Assist Prof
DAIYASU, Hiromi
(D Sc)

Vis Assist Prof
ICHIHARA, Hisako

PD
HOSHIYAMA, Daisuke
(D Sc)

PD
KATOH, Kazutaka
(D Sc)

PD
KOJIMA, Kenji
(Ph D)

PD
NEMOTO, Wataru
(D Sc)

Student

SATO, Tetsuya (D2)

Scope of Research

Evolutionary studies based on molecular biology is called “molecular evolutionary biology”, which is one of the origins of the current bioinformatics. Living organisms have acquired wide variety of functions during the course of the evolution by changing the information encoded by the genomes. Inversely, reconstruction of the evolutionary history related to the functions would bring us a great insight into the acquired functions and the life. Furthermore, such evolutionary information is useful for practical fields such as drug design and proteins engineering. We develop new methodologies with evolutionary information, to extract biological knowledge from various molecular biological data including sequence and structure data of individual genes and proteins, genome data, and expression profile data. We also analyze the data of molecular biology from the evolutionary viewpoint, to obtain novel biological knowledge.

Research Activities (Year 2005)

Presentations

Computational Analysis of Substrate Specificity of Disaccharide-Specific Glycosidase., Daiyasu H, Mizutani M, Saitoh H, Sakata K, Toh H (Medical Institute of Bioregulation, Kyushu University), 5th Annual Metting of Protein Science Society of Japan, 30 June.

Evolutionary Analysis of Proteins Relevant to Quorum sensing., Ichihara H, Kuma K, Toh H (Medical Institute of Bioregulation, Kyushu University), 5th Annual Metting of Protein Science Society of Japan, 1 July.

Improvement in the Accuracy of Multiple Sequence Alignment Program MAFFT., Katoh K, Kuma K, Miyata T (JT Biohistory Resarch Hall, Waseda University), and Toh H (Medical Institute of Bioregulation, Kyushu University), 5th Int’l Workshop on Bioinformatics and Systems Biology, 22 August, Berlin.

Construction of Phylogenetic Tree Database for the Gene Families Involved in the Signal Transduction., Kuma K, Hirose N (Graduate School of Science, Kyoto University), Toh H (Medical Institute of Bioregulation, Kyushu University), Iwabe N (Graduate School of Science, Kyoto University), The 28th Annual Meeting of the Molecular Biology Society of Japan, 7 December.

Dualen: An Extraordinary Non-LTR Retrotransposon Family Encoding Dual Endonucleases., Kojima K, Fujiwara H (University of Tokyo), 77th Annual Meeting of the Genetics Society of Japan, 28 September.

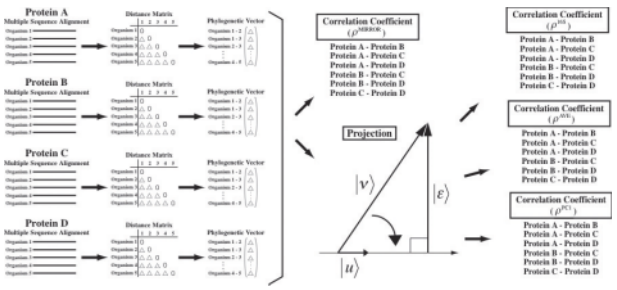
Comparison of Prediction Methods for Protein-Protein Interactions Using Co-evolutionary Information., Sato T, Yamanishi Y (Centre de Geostatistique , Ecole des Mines de Paris), Ichihara H, Kanehisa M, Toh H (Medical Institute of Bioregulation, Kyushu Univ.), 16th International Conference on Genome Informatics (GIW2005), 19 - 21 December.

Topics

The former Professor Hiroyuki Toh resigned on 31 March 2005.

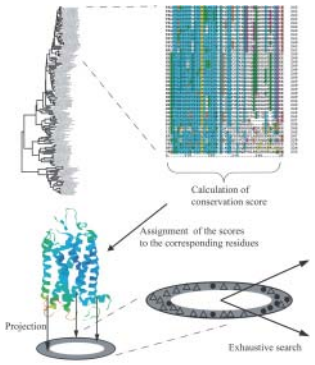
The Inference of Protein-Protein Interactions by Co-evolutionary Analysis is Improved by Excluding the Information about the Phylogenetic Relationships

The prediction of protein-protein interactions is currently an important issue in bioinformatics. The mirror tree method uses evolutionary information to predict protein-protein interactions. However, it has been recognized that predictions by the mirror tree method lead to many false positives. The incentive of our study was to solve this problem by improving the method of extracting the co-evolutionary information regarding the protein pairs. We developed a novel method to predict protein-protein interactions from co-evolutionary information in the framework of the mirror tree method. The originality is the use of the projection operator to exclude the information about the phylogenetic relationships among the source organisms from the distance matrix. Each distance matrix was transformed into a vector for the operation. The vector is referred to as a 'phylogenetic vector'. We have proposed three ways to extract the phylogenetic information: (1) using the 16S rRNA from the same source organisms as the proteins under consideration, (2) averaging the phylogenetic vectors and (3) analyzing the principal components of the phylogenetic vectors. We examined the performance of the proposed methods to predict interacting protein pairs from *Escherichia coli*, using experimentally verified data. Our method was successful, and it drastically reduced the number of false positives in the prediction.



Prediction of Interfaces for Oligomerizations of G-protein Coupled Receptors

Several lines of biochemical and pharmacological evidence have suggested that some G-protein coupled receptors (GPCRs) form homo oligomers, hetero oligomers or both. The GPCRs oligomerizations are considered to be related to signal transduction and some diseases. Therefore, an accurate prediction of the residues that interact upon oligomerization interface would further our understanding of signal transduction and the diseases in which GPCRs are involved. One of the complications for such a prediction is that the interfaces differ with the subtypes, even within the same GPCR family. Focusing on the distribution of residues conserved on the molecular surface in a particular subtype, we developed a new method to predict the interface for the GPCR oligomers, and applied it to several subtypes of known GPCRs to check the sensitivity. Subsequently, we found that predicted interfaces of rhodopsin, D_2 dopamine receptor and b_2 adrenergic receptor agreed with the experimentally suggested interfaces, despite difference in the interface region among the three subtypes. Moreover, a highly conserved residue detected from the D_2 dopamine receptor corresponded to a residue involved in a missense change found in the large family of myoclonus dystonia. Our observation suggests the possibility that the disease is caused by the disorder of the oligomerization, although the molecular mechanism of the disease has not been revealed yet. The benefits and the pitfalls of the new method will be discussed, based on the results of the applications.



Grants

Kuma K, A Study of Relationship between Mammalian Specific Features and Gene Diversification on the Basis of Genome Comparisons., Grant-in-Aid for Scientific Research (C), April 2005 - March 2007.

Kojima K, Acquiring New Function and the Evolution of Survival Strategy of Non-LTR Retrotransposons, Grant-in-Aid for Scientific Research for JSPS Researcher, 1 April 2005 - 31 March 2006.

Awards

Nemoto W and Toh H, Award in The 14th ScreenTech & TargetTalk 2005, Prediction of GPCR Oligomer Interface, IBC Life Sciences, 21 - 23 March, USA.

Nemoto W and Toh H, Poster Award in Int'l Biophysics Congress, Prediction of Interfaces for Oligomerization of GPCRs, IUPAB & EBSA & SFB & CNB, 28 August - 1 September, France.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
KIRA, Mitsuo
(D Sc)

Laboratory of Organoelement Chemistry
Professor, Department of Chemistry, Graduate School of Science, Tohoku University
(Aoba-ku, Sendai 980-8578)

Lecture at *ICR*
Can Silicon Chemistry Surpass Organic Chemistry?

Vis Prof
TABATA, Satoshi
(D Sc)

Laboratory of Molecular Biology
Vice-Director, Kazusa DNA Research Institute
(1532-3 Yanauchino, Kisarazu 292-0821)

Lecture at *ICR*
Genomics on Flowering Plants (*Arabidopsis thaliana, Lotus japonicus*) and Plant-related Microbes (cyanobacteria and rhizobia)

Vis Prof
NISHIO, Taichi
(D Eng)

Laboratory of Polymer Materials Science
Vice President, Sanzen Kako Co. Ltd.
(Toyocho Sinnei Building 9 th floor, 1-3-4 Toyo Koto-ku, Tokyo 135-0016)

Lecture at *ICR*
Present Situation and Vision for Polyolefin as a Background of Social Environment

Vis Prof
NAGASHIMA, Hideo
(D Eng)

Laboratory of Organotransition Metal Chemistry
Professor, Applied Molecular Chemistry and Analytical Center in Institute for Materials Chemistry and Engineering, Graduate School of Engineering Sciences, Kyushu University
(Kasuga, Fukuoka 816-8580)

Lecture at *ICR*
Organometallic Chemistry on Ruthenium Clusters: Specific Activation of Hydrosilylation and Application to Catalytic Reactions for the Synthesis of Organic Compounds and Polymers

Vis Prof
ATTFIELD, John Paul
(Ph D)

Laboratory of Advanced Solid State Chemistry
Professor of Materials Science at Extreme Conditions, University of Edinburgh
(School of Chemistry, Joseph Black Building, West Mains Road, Edinburgh, Scotland EH9 3JJ, UK)

Lecture at *ICR*
The Chemical Control of Electron Oxides

Vis Prof
WANG, Yu
(Ph D)

Laboratory of Organotransition Metal Chemistry
Professor, Department of Chemistry, National Taiwan University
(No.1 Sec. 4, Roosevelt Road, Taipei, Taiwan)

Lecture at *ICR*
Spin Transition and LIESST Phenomena of Fe(II) Complexes

Vis Assoc Prof
KATO, Atsushi
(D Sc)

Laboratory of Chemistry of Polymeric Functionality Materials
Senior Researcher, Research Department, Nissan Arc, Ltd.
(1, Natsushima-cho, Yokosuka 237-0061)

Lecture at *ICR*
Analysis of Ruptured Surface and Cross Section of Polymeric Materials

Vis Assoc Prof
MORITA, Akihiro
(D Sc)

Laboratory of Solution and Interface Chemistry
Assoc Prof, Department of Computational Molecular Science, Institute for Molecular Science
(Meidaijicho, Okazaki 444-8585)

Lecture at *ICR*
High-Resolution Quantum Study of Molecular Structure and Interaction of Liquid Surface

Vis Assoc Prof
TSUKISHIMA, Chihiro
(D Eng)

Laboratory of Laser Matter Interaction Science
High Frequency Electro-magnetics Group Manager, Advanced R&D Center, Mitsubishi Electric Corporation
(8-1-1 Tsukaguchi-honmachi, Amagasaki 661-0001)

Lecture at *ICR*
Present and Future of Particle Cancer-therapy Facility Sterilization with Electron Beam

Vis Assoc Prof
MARUYAMA, Osamu
(D Sc)

Laboratory of Biological Information Networks
Associate Professor, Faculty of Mathematics, Kyushu University
(6-10-1, Hakozaki, Higashi-ku, Fukuoka 812-8581)

Lecture at *ICR*
Reconstructing Phylogenetic Trees of Prokaryote Genomes by Randomly Sampling Oligopeptides

PERSONAL

Retirement

Professor KOMATSU, Koichi

(Structural Organic Chemistry, Division of Synthetic Chemistry)

On March 31st, 2006, Dr. Koichi Komatsu retired from Kyoto University after 35 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Komatsu was born in Kyoto on May 24th, 1942. After spending one year at Davidson College, USA, as a Richardson Scholar, he graduated from Faculty of Engineering, Kyoto University, in 1966. He studied mechanisms of carbocation reactions at the Graduate School of Engineering under the supervision of Professor Kunio Okamoto, and was granted a doctoral degree with a thesis titled "Mechanistic Study on the One-Electron Reduction of Carbonium Ions" in 1974. In 1971, he was appointed an Assistant Professor of Department of Hydrocarbon Chemistry, at the Graduate School of Engineering, Kyoto University. On leave from Kyoto University from 1974 to 1976, he studied synthesis and properties of electron-deficient π-conjugated systems, polyquinocyclopropanes, in the laboratory of Professor Robert West at the University of Wisconsin, Madison, as a postdoctoral research associate. Dr. Komatsu was promoted to a Lecturer in 1984 and to an Associate Professor in 1989 in the School of Engineering, Kyoto University. In 1993 he moved to Institute for Chemical Research, where he was promoted to a full Professor in 1995 and directed the Laboratory of High-Pressure Organic Chemistry (presently re-named Structural Organic Chemistry).

Throughout his academic career, Dr. Komatsu has devoted himself to the fundamental studies on two- and three-dimensional π-conjugated compounds, pursuing the creation of organic π-systems with ultimate novelty in their structures as well as their properties.

His research subjects, carried out based on his firm background of physical organic chemistry, are classified into three major themes, that is, super-stabilization of organic cationic species, creation of π-conjugated systems with novel structures, and organic chemistry of fullerenes.

In the first two themes, he found that the combined use of σ-π conjugation and steric protection by bicycloalkene units entirely surrounding cyclic π-systems is highly effective for realization of organic compounds with novel electronic structures, which could have never been attained by any other conventional method. Thus, various types of carbocations and radical cations with a broad structural range, possessing extraordinary stability have been synthesized, together with novel cyclic π-systems with unusual bond alternation.

In the third theme, Dr. Komatsu also made great achievements, which are now widely recognized as landmarks in the development of fullerene chemistry. First, by his invention of the mechanochemical solid-state reaction, he succeeded in the first and highly selective synthesis of dumbbell-shaped fullerene dimer, C_{120}. This achievement was followed by the discovery of efficient cage opening and closing reactions on fullerenes, which led to the success of the first organic synthesis of endohedral fullerenes encapsulating molecular hydrogen in a macroscopic amount.

These achievements, which are results of the contribution of his dedicated colleagues and students, have been published as 223 original articles in international journals and 34 accounts and reviews.

For these distinguished accomplishments, he was honored with The Divisional Award of The Chemical Society of Japan for 1998 (Organic Chemistry), Alexander von Humboldt Research Award in 2002, and The Chemical Society of Japan Award for 2005.

His contribution to Kyoto University through his scientific and educational activities is hereby gratefully acknowledged. His warm and sincere personality will remain deep in the hearts of his colleagues and students.

Retirement

Professor KOHJIYA, Shinzo

(Chemistry of Polymeric Functionality Materials,
Division of Materials Chemistry)

On 31st of March 2006, Dr. Shinzo Kohjiya retired from Kyoto University after 13 years of service. Dr. Kohjiya was born in Osaka on December 23, 1942. He graduated from Department of Polymer Chemistry, Faculty of Engineering, Kyoto University in 1965. He started his research carrier on kinetic study of ionic polymerization in Graduate School of Engineering, Kyoto University under the supervision of late Professor S. Okamura. After completing his Master's degree in 1967, he proceeded to the doctoral program. During the doctoral study, in 1969, he was appointed as an Instructor of Faculty of Engineering and Design, Kyoto Institute of Technology. He continued his study and was granted a doctoral degree for a thesis entitled "Kinetic studies on the cationic polymerization of cyclic dienes" in 1975. In 1977, he was promoted to an Associate Professor, and in 1991, to a full Professor, of Faculty of Engineering and Design, Kyoto Institute of Technology. On leave from Kyoto Institute of Technology, from 1978 to 1979, he studied on chemistry of calixarenes under Professor C. David Gutsche at Department of Chemistry, Washington University in St. Louis as a Research Associate. In 1993, he was transferred to Institute for Chemical Research, Kyoto University.

During his academic carrier, Dr. Kohjiya devoted himself to the studies on synthesis, modification, analysis and characterization of elastomer and rubbery materials. He started his study from determination of rate constants in ionic polymerization of dienes, especially cyclic diens such as cyclopentadiene. Then, he extended his field of study to the fabrication of functional diene polymers and their cross-linking reactions. He synthesized novel ionene elastomers which posess ionic groups, and investigated the relationship between their structures and properties. He studied also on polyurethane elastomers, and on the basis of these studies, he developed functionality elastomers having blood compatibility or ionic conductivity.

He further extended his focus of research to fundamental understanding of elastomeric properties of polymer network systems. He investigated the structural changes during the process of gelation from chemical and structural viewpoints, and presented significant results in terms of the relationship between the chemical cross-linking and physical entanglement. He contributed also for the understanding of filler reinforcement of rubber materials, which is important from both industrial and scientific viewpoints. He developed the in-situ silica formation technique, which utilized the sol-gel reaction in a rubber matrix. This technique enabled silica particles with controlled size to accomplish the better dispersion using the lower energy. He also studied on the strain-induced crystallization, which is regarded as smart in-situ nano-compounding. In his recent work, he applied the electron tomography to the analysis of three-dimensional dispersion of carbon black particles in the natural rubber matrix, and presented significant results concerning the effect of dispersion of nanoscopic particles on physical properties. For the contribution of his works to the rubber science, he received, in 1987, the Best Paper Award from the Society of Rubber Industry, Japan, and in 1994, The Oenslager Award from the Chemical Society of Japan and the Society of Rubber Industry, Japan.

He gave many lectures in Kyoto University and Kyoto Institute of Technology, and supervised the dissertation works of graduate students. From 1998 to 1999, he served as the president of the Society of Rubber Industry, Japan. He served also as a member or a chairman of several international conferences on the rubber science.

His contribution to Kyoto University through both Scientific and educational activities is hereby greatly acknowledged.

Awards

TAKANO, Mikio　IKEDA, Yasunori

The L'Oreal Art & Science of Color Prizes, The 8th Gold Prize

"Microstructure and Formation Process of the Characteristic Reddish Color Pattern 'Hidasuki' on Bizen Stoneware:Reactions Involving Rice Straw"

The L'Oreal Art & Science Foundation

21 October 2005

TAKEDA, Nobuhiro

The ICR Award for Young Scientists

"Synthesis of Novel Organosilicon Species by Taking Advantage of a Silylene Bearing Bulky Substituents and the Elucidation of Their Properties"

ICR

2 December 2005

SASAMORI, Takahiro

Inoue Research Award for Young Scientists

"Studies on the Synthesis of Low-coordinated Species of Heavier Group 15 Elements Utilizing Kinetic Stabilization"

Inoue Foundation for Science

4 February 2005

MURATA, Michihisa

The Best Oral Presentation Award

The 85th Annual Meeting of the Chemical Society of Japan

"The First Synthesis of Fullerene C_{60} Encapsulating Molecular Hydrogen"

The Chemical Society of Japan　27 March 2005

The ICR Award for Students

"Organic Synthesis of Fullerene C_{60} Encapsulating Molecular Hydrogen"

ICR　2 December 2005

AZUMA, Masaki

Young Scientists' Prize, the Commendation for Science and Technology

"Study of Functional Oxides by High-Pressure Synthesis in The Field of Solid State Chemistry"

MEXT

20 April 2005

TSUJII, Yoshinobu

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

"Studies on Precise Surface Modification by Living Radical Polymerization"

The Society of Fiber Science and Technology, Japan

8 July 2005

ONO, Teruo

Marubun Academic Award

"Study on Dynamics of a Magnetic Domain Wall in Magnetic Nanowire for Spintronic Device Application"

Marubun Research Promotion Foundation

7 March 2005

KATO, Utako

Inoue Research Award for Young Scientists

"Regulation of Phospholipid Translocation Across the Plasma Membrane and Its Role for Cell Polarity Formation in Saccharomyces Cerevisiae"

Inoue Foundation for Science

4 February 2005

FUKAZAWA Aiko

The Best Oral Presentation Award

The 85th Annual Meeting of the Chemical Society of Japan

"Perfect all-anti Oligosilanes: Conformation Control of Oligosilanes Utilizing Bicyclic Trisilane Units"

The Chemical Society of Japan

27 March 2005

SAITO, Takashi

Encouragement Prize of the Japan Society of High Pressure Science and Technology

"Search of Transition Metal Oxides and Development of Single Crystal Growth Technique Using High Pressure Method"

The Japan Society of High Pressure Science and Technology

30 October 2005

KAN, Daisuke

The ICR Award for Students

"Blue-Light Emission at Room Temperature from Ar^{+}-Irradiated $SrTiO_3$"

ICR

2 December 2005

KANEMITSU, Yoshihiko

The Ichimura Prize

"Pioneering Contributions for Light Emitting Nanoparticles"

The New Technology Development Foundation

28 April 2005

Paper Awards

SHINOHARA, Akihiro; TAKEDA, Nobuhiro; SASAMORI, Takahiro; TOKITOH, Norihiro

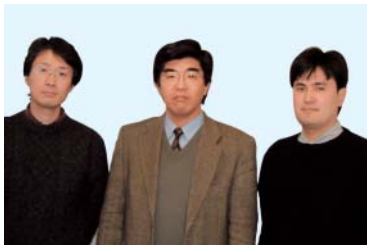
The BCSJ Award (The Best Article of the Month)

Bulletin of the Chemical Society of Japan, **78**, 977-987 (2005).

"Synthesis of Kinetically Stabilized 1-Silanaphthalenes and Their Properties"

The Chemical Society of Japan

15 June 2005



HAINO, Takeharu[1]; SEYAMA, Jun[1]; FUKUNAGA, Chigusa[1]; MURATA, Yasujiro; KOMATSU, Koichi; FUKAZAWA, Yoshimasa[1]

The BCSJ Award (The Best Article of the Month)

Bulletin of the Chemical Society of Japan, **78**, 768-770 (2005).

"Calix[5]arene-Based Receptor for Dumbbell-Shaped C_{120}"

The Chemical Society of Japan

15 May 2005

[1] Hiroshima University

YOSHIDA, Yukihiro[1]; OTSUKA, Akihiro[1,2]; SAITO, Gunzi[1]; NATSUME, Seiichi[3]; NISHIBORI, Eiji[3]; TAKATA, Masaki[4]; SAKATA, Makoto[3]; TAKAHASHI, Masahide; YOKO, Toshinobu

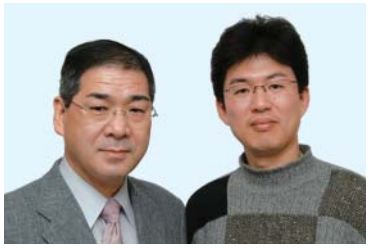
The BCSJ Award (The Best Article of the Month)

Bulletin of the Chemical Society of Japan, **78**, 1921-1928 (2005).

"Conducting and Magnetic Properties of 1-Ethyl-3-methylimidazolium (EMI) Salts Containing Paramagnetic Irons: Liquids [EMI][$M^{III}Cl_4$] (M = Fe and $Fe_{0.5}Ga_{0.5}$) and Solid [EMI]$_2$[$Fe^{II}Cl_4$] "

The Chemical Society of Japan

15 November 2005



[1] Graduate School of Science, Kyoto University, [2]Research Center for Low Temperature and Materials Sciences, Kyoto University, [3]Nagoya University, [4] Japan Synchrotron Radiation Research Institute (JASRI)

Poster Awards

MIZUHATA, Yoshiyuki

The Best Poster Award

The 10th Symposium of the Society of Silicon Chemistry

"Synthesis of a Stable 2-Stannanaphthalene and Its Structure and Properties"

The Society of Silicon Chemistry, Japan

28 October 2005

MURATA, Michihisa

Student Poster Award

PACIFICHEM 2005

"Organic Synthesis of Endohedral C_{60} Encapsulating Molecular Hydrogen, $H_2@C_{60}$"

18 December 2005

MAEDA, Shuhei

Student Poster Award

PACIFICHEM 2005

"Synthesis of Open-Cage C_{70} and Encapsulation of Molecular Hydrogen inside the Cage"

18 December 2005

TANIMA, Daisuke

Best Poster Award

11th Summer Meeting of Functional Host-Guest Chemistry

"Temperature-Dependent Coloration of Functional Phenolphthalein Derivatives"

28 July 2005

MONGUCHI, Daiki

Best Poster Award

25th Seminar on Synthetic Organic Chemistry for Young Scientists

"Asymmetric Intramolecular Conjugate Addition of Chiral Enolates via Racemization-Free Equilibrium"

The Society of Synthetic Organic Chemistry of Japan, Kansai Branch

24 November 2005

TAKAISHI, Kazuto

Best Poster Award

25th Seminar on Synthetic Organic Chemistry for Young Scientists

"Fine Organic Synthesis of Chiral Oligonaphthalenes"

The Society of Synthetic Organic Chemistry of Japan, Kansai Branch

24 November 2005

MAEDA, Takahiro

Poster Award

6th Pacific Rim Conference on Ceramic and Glass Technology

"Fabrication of TiO_2 Periodic Structure by the Photopolymerization-Induced Phase Separation Method"

The American Ceramic Society

12 September 2005

FUKAZAWA, Aiko

Award for the First Place Poster Contribution

The 14th International Symposium on Organosilicon Chemistry

"all-anti Oligosilanes: Conformation Control of Oligosilanes Utilizing the Bicyclic Trisilane Unit"

5 August 2005

Student Poster Award

PACIFICHEM 2005

"Perfect all-anti Oligosilanes: Conformation Control of Oligosilanes Utilizing the Bis(tetramethylene)-tethered Bicyclic Trisilane Unit"

18 December 2005

NEMOTO, Wataru; TOH, Hiroyuki[1]

Poster Award

The 14th ScreenTech & TargetTalk 2005

"Prediction of GPCR oligomer interface"

IBC Life Sciences

23 March 2005

Poster Award

Int'l Biophysics Congress

"Prediction of Interfaces for oligomerization of GPCRs"

The Int'l Union of Pure and Applied Biophsics (IUPAB) & European Biophysical Societies' Association (EBSA) & The Societe Francaise de Biohysique(SFB) & Comite National de Biophysique (CNB)

1 September 2005

[1] Kyushu University

PUBLICATIONS

INTERNATIONAL RESEARCH COLLABORATIONS

THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

Saito M, Tokitoh N, Okazaki R: Tin-Chalcogen Double-Bond Compounds, Stannanethione and Stannaneselone: Synthesis, Structure, and Reactivities, *J. Am. Chem. Soc*., **126**, 15572-15582 (2004).

Sasamori T, Mieda E, Nagahora N, Takeda N, Takagi N, Nagase S, Tokitoh N: Systematic Studies on Redox Behavior of Homonuclear Double-bond Compounds of Heavier Group 15 Elements, *Chem. Lett*., **34**, 166-167 (2005).

Sasamori T, Sasaki T, Takeda N, Tokitoh N: Reactions of a Germacyclopropabenzene with Elemental Chalcogens: Syntheses and Structures of a Series of Stable *2H*-Benzo[c][1,2]chalcogenagermetes, *Organometallics*, **24**, 612-618 (2005).

Tajima T, Sasaki T, Sasamori T, Takeda N, Tokitoh N: Reactivities of Germacyclopropabenzene toward Some Transition Metal Carbonyl Complexes, *Appl. Organometal. Chem*., **19**, 570-577 (2005).

Tokitoh N, Shimizu D, Takeda N, Sasamori T: Syntheses of Polythioethers Tethered with Bulky Aryl Groups and Their Complexation with Late-Transition Metals, *Phosphorus, Sulfur and Silicon*, **180**, 1241-1245 (2005).

Sasamori T, Mieda E, Takeda N, Tokitoh N: Telluradistibirane and Telluradibismirane: Three-Membered Heterocycles of Heavier Main Group Elements, *Angew. Chem. Int. Ed*., **44**, 3717-3720 (2005).

Shinohara A, Takeda N, Sasamori T, Tokitoh N: Synthesis of Kinetically Stabilized 1-Silanaphthalenes and Their Properties, *Bull. Chem. Soc. Jpn*., **78**, 977-987 (2005).

Nagahora N, Sasamori T, Takeda N, Tokitoh N: Synthesis and Structure of a Stable 1,3-Dihydrotriphosphane and Its Thermal Decomposition Leading to the Formation of the Corresponding Phosphine and Diphosphene, *Organometallics*, **24**, 3074-3080 (2005).

Sasamori T, Sugiyama Y, Takeda N, Tokitoh N: Structure and Properties of an Overcrowded 1,2-Dibromodigermene, *Organometallics*, **24**, 3309-3314 (2005).

Takeda N, Shimizu D, Sasamori T, Tokitoh N: Dichloro[1,2-bis(phenylsulfanyl)benzene]palladium(II), *Acta Cryst. E*, **61**, m1408-m1410 (2005).

Mizuhata Y, Takeda N, Sasamori T, Tokitoh N: Generation of 9-Stannaphenanthrene and Its Reactivities, *Chem. Lett*., **34**, 1088-1089 (2005).

Tajima T, Takeda N, Sasamori T, Tokitoh N: Generation and Reactions of Overcrowded Diaryldilithiostannane and Diaryldipotassiostannane, *Eur. J. Inorg. Chem*., **2005**, 4291-4300 (2005).

Takeda N, Shimizu D, Tokitoh N: Synthesis and Structure of a Distorted Octahedral Palladium(II) Complex Coordinated with a New Tetrathioether Ligand Tethered with Bulky Substituents, *Inorg. Chem*., **44**, 8561-8568 (2005).

Sasamori T, Tokitoh N: Group 14 Multiple Bonding, *In Encyclopedia of Inorganic Chemistry, 2nd Edition, Ed by R. Bruce King, John Wiley & Sons*, 1698-1740 (2005).

Mizuhata Y, Sasamori T, Takeda N, Tokitoh N: Synthesis and Properties of a Stable 6-Stannapentafulvene, *Chem. Commun*., **2005**, 5876-5878 (2005).

Shinohara A, Takeda N, Sasamori T, Matsumoto T, Tokitoh N: Synthesis and Properties of η^6-Silabenzene-M(CO)$_3$ Complexes (M= Cr and Mo), *Organometallics*, **24**, 6141-6146 (2005).

Matsuda T, Tsuji K, Kamitanaka T, Harada T, Nakamura K, Ikariya T: Rate Enhancement of Lipase-Catalyzed Reaction in Supercritical Carbon Dioxide, *Chem. Lett*., **34**, 1102-1103 (2005).

Matsuda T, Harada T, Nakamura K, Ikariya S: Asymmetric Synthesis Using Hydrolytic Enzymes in Supercritical Carbon Dioxide, *Tetrahedron:Asymm*, **16**, 909-915 (2005).

Matsuda T, Harada T, Nakamura K: Biocatalysis in Supercritical CO2, *Current Organic Chemistry*, **9**, 299-315 (2005).

Itoh K, Sakamaki H, Nakamura K, Horiuchi A: Biocatalytic Symmetric Reduction of 3-acetylisoxazoles, *Tetrahedron: Asymmetry*, **16**, 1403-1408 (2005).

Albrycht M, Kielbasinski P, Drabowicz J, Mikolajczyk M, Matsuda T, Nakamura K: Supercritical Carbon Dioxide as a Reaction Medium for Enzymatic Kinetic Resolution of P-chiral Hydroxymethanephosphinates, *Tetrahedron: Asymmetry*, **16**, 2015-2018 (2005).

Matsuda T, Nakamura K: Asymmetric Synthesis Using Biocatalysts, *Chiral Chemistry-Asymmetric Synthesis, Maruzen*, 127-153 (2005).

Matsuda T, Nakamura K: Enzymatic Reactions, *A Handbook for Chemistry, Fundamental Part, 5th Ed, Maruzen*, II-539-547 (2004).

— Structural Organic Chemistry —

Nishinaga T, Uto T, Komatsu K: Novel Cyclooctatetraene Radical Cation Planarized by Full Annelation with Bicyclo [2.1.1]hexene Units, *Org. Lett*., **6**, 4611-4613 (2004).

Yamazaki T, Murata Y, Komatsu K, Furukawa K, Morita M, Maruyama N, Yamao T, Fujita S: Synthesis and Electrolytic Polymerization of the Ethylenedioxy-Substituted Terthiophene-Fullerene Dyad, *Org. Lett*., **6**, 4865-4868 (2004).

Ishida S, Nishinaga T, West R, Komatsu K: Generation and Aromaticity of 2-Silaimidazolium Ion, a New π-Conjugated Silylium Ion, *Chem. Commun*., 778-780 (2005).

Stanisky C M, Cross R J, Saunders M, Murata M, Murata Y, Komatsu K: Helium Entry and Escape through a Chemically Opened Window in a Fullerene, *J. Am. Chem. Soc*., **127**, 299-302 (2005).

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

Kitagawa T, Lee Y, Masaoka N, Komatsu K: Generation and Properties of a Novel Alkylated C_{70} Cation, *Angew. Chem. Int. Ed*., **44**, 1398-1401 (2005).

Sawa H, Wakabayashi Y, Murata Y, Murata M, Komatsu K: Floating Single Hydrogen Molecule in an Open-Cage Fullerene, *Angew. Chem. Int. Ed*., **44**, 1981-1983 (2005).

Miyata Y, Nishinaga T, Komatsu K: Synthesis and Structural, Electronic, and Optical Properties of Oligo(thienylfuran)s in Comparison with Oligothiophenes and Oligofurans, *J. Org. Chem*., **70**, 1147-1153 (2005).

Ishida S, Nishinaga T, Komatsu K: The First Isolation of 1,3-Diaza-2-sila-4-cyclopentene Radical Cation Salt: The X-ray Structure and Electronic Properties, *Chem. Lett*., **34**, 486-487 (2005).

Frankevich V E, Dashtiev D, Zenobi R, Kitagawa T, Lee Y, Murata Y, Yamazaki T, Gao Y, Komatsu K, Oliva J M: MALDI-Fourier Transform Mass Spectrometric and Theoretical Studies of Donor-Acceptor and Donor-Bridge-Acceptor Fullerenes, *Phys. Chem. Chem. Phys*., **7**, 1036-1042 (2005).

Wang G-W, Chen A-X, Murata Y, Komatsu K: [60]Fullerene Adducts with 9-Substituted Anthracenes: Mechanochemical Preparation and Retro Diels-Alder Reaction, *Tetrahedron*, **61**, 4851-4856 (2005).

Yoshimoto S, Honda Y, Murata Y, Murata M, Komatsu K, Ito O, Itaya K: Dependence of Molecular Recognition of Fullerene Derivative on the Adlayer Structure of Zinc Octaethylporphyrin Formed on Au(100) Surface, *J. Phys. Chem. B*, **109**, 8547-8550 (2005).

Haino T, Seyama J, Fukunaga C, Murata Y, Komatsu K, Fukazawa Y: Calix[5]arene-based Receptor for Dumbbell-Shaped C_{120}, *Bull. Chem. Soc. Jpn*., **78**, 768-770 (2005).

Horie R, Araki Y, Ito O, Lee Y, Kitagawa T, Komatsu K: Study of Photoinduced Electron Transfer between [60]Fullerene and Proton-sponge by Laser Flash Photolysis: Addition Effects of Organic Acid, *J. Phys. Chem. A*, **109**, 6140-6146 (2005).

Uto T, Nishinaga T, Matsuura A, Inoue R, Komatsu K: A Naphthalene with Unusual Bond Alternation Made by Annelation with Bicyclo[2.1.1]hexene Units: Aromaticity and Reactivity, *J. Am. Chem. Soc*., **127**, 10162-10163 (2005).

Ogawa K, Kitagawa T, Ishida S, Komatsu K: Synthesis and Structure of a New Silver(I) Salt of the Tetrakis(pentafluorophenyl)borate Anion with Novel Tris η^1-benzene Coordination, *Organometallics*, **24**, 4842-4844 (2005).

Komatsu K, Nishinaga T: Synthesis and Properties of Cationic π-Conjugated Systems Stabilized by Bicyclo[2.2.2]octene Units, *Synlett*, 187-202 (2005).

Nishinaga T, Komatsu K: Persistent π Radical Cations: Self-association and Its Steric Control in Condensed Phase, *Org. Biomol. Chem*., **3**, 561-569 (2005).

Komatsu K: The Mechanochemical Solid-State Reaction of Fullerenes, *Top. Curr. Chem*., **254**, 185-206 (2005).

Komatsu K, Murata Y: A New Route to an Endohedral Fullerene by Way of σ-Framework Transformations, *Chem. Lett. (Highlight Review)*, **34**, 886-891 (2005).

Sato H, Tashiro K, Shinmori H, Osuka A, Murata Y, Komatsu K, Aida T: Positive Heterotropic Cooperativity for Selective Guest Binding via Electronic Communications through a Fused Zinc Porphyrin Array, *J. Am. Chem. Soc*., **127**, 13086-13087 (2005).

Komatsu K: 100% Storage of Hydrogen in Fullerene, *Collection of Hydrogen Utilization Technique, Bookers*, **2**, 223-228 (2005) (in Japanese).

Komatsu, K: First Chemical Synthesis of $H_2@C_{60}$, *Electronic Properties of Novel Nanostructures, AIP, NY,* **XIX**, 50-55 (2005).

Matsuo Y, Isobe H, Tanaka T, Murata Y, Murata M, Komatsu K, Nakamura E: Organic and Organometallic Derivatives of Dihydrogen-Encapsulated [60]Fullerene, *J. Am. Chem. Soc*., **127**, 17148-17149 (2005).

Cheng X, Wang G-W, Murata Y, Komatsu K: Solvent-Free Synthesis of Dihydrofuran-Fused [60]Fullerene Derivatives by High-Speed Vibration Milling, *Chin. Chem. Lett*., **16**, 1327-1329 (2005).

— Synthetic Organic Chemistry —

Kawabata T, Majumdar S, Tsubaki K, Monguchi D: Memory of Chirality in Intramolecular Conjugate Addition of Enolates: A Novel Access to Nitrogen Heterocycles with Contiguous Quaternary and Tertiary Stereocenters, *Org. Biomol. Chem*., **3**, 1609-1611 (2005).

Kawabata T, Chen J, Suzuki H, Fuji K: Stereochemical Study on α-Alkylation of β-Blanched α-Amino Acid Derivatives via Memory of Chirality, *Synthesis*, 1368-1377 (2005).

Tsubaki K, Kusumoto T, Hayashi N, Tanima D, Fuji K, Kawabata T: Convenient Preparation of Optically Active *N,N*-Bis(4-substituted-4-aminobutyl)amines, *Tetrahedron: Asymmetry*, **16**, 739-743 (2005).

Tsubaki K, Tanima D, Nuruzzaman M, Kusumoto T, Fuji K, Kawabata T: Visual Enantiomeric Recognition of Amino Acid Derivatives in Protic Solvents, *J. Org. Chem*., **70**, 4609-4616 (2005).

Tsubaki K: Synthesis and Properties of Homooxacalix[3]arenes, *New Trend in Structural Organic Chemistry*, 61-83 (2005).

— Advanced Inorganic Synthesis —

Masuno A, Terashima T, Takano M: Epitaxial Growth of Perovskite-Type $LaVO_3$ Thin Films on Various Substrates by the PLD Method, *Solid State Ionics*, **172**, 275-278 (2004).

Shen K M, Yoshida T, Lu D H, Ronning F, Armitage N P, Lee W S, Zhou X J, Damascelli A, Feng D L, Ingle N J C, Eisaki H, Kohsaka Y, Takagi H, Kakeshita T, Uchida S, Mang P K, Greven M, Onose Y, Taguchi Y, Tokura Y, Komiya S, Ando Y, Azuma M, Takano M, Fujimori A, Shen Z-X: Fully Gapped Single-Particle Excitations in Lightly Doped Cuprates, *Phys. Rev. B*, **69**, [054503-1]-[054503-5] (2004).

Masuno A, Terashima T, Shimakawa Y, Takano M: Current-Induced Electroresistive Effect in Mixed-Phase $La_{0.67}Ca_{0.33}MnO_3$ Thin Films, *Appl. Phys. Lett*., **85**, 6194-6196 (2004).

Waku K, Katsufuji T, Kohsaka Y, Sasagawa T, Takagi H, Kishida H, Okamaoto H, Azuma M, Takano M: Charge Dynamics of $Ca_{2-x}Na_xCuO_2Cl_2$ as a Correlated Electron System with the Ideal Tetragonal Lattice, *Phys. Rev. B*, **70**, [134501-1]-[134501-8] (2004).

Azuma M, Kohsaka Y, Yamada I, Belik A A, Takagi H, Takano M: Single-Crytal Growth and New-Material Search for Oxides at High Pressures, *Oyobutsuri*, **74**, 27-31 (2005) (in Japanese).

Shen K M, Ronning F, Lu D H, Baumberger F, Ingle N J C, Lee W S, Meevasana W, Kohsaka Y, Azuma M, Takano M, Takagi M, Shen Z-X: Nodal Quasiparticles and Antinodal Charge Ordering in $Ca_{2-x}Na_xCuO_2Cl_2$, *Science*, **307**, 901-904 (2005).

Yu R, Xing X, Saito T, Azuma M, Takano M, Wang D, Chen Y, Kumada N, Kinomura N: A Novel Organically Templated Hybrid Open-Framework Manganese Phosphate-Oxalate, *Solid State Sciences*, **7**, 221-226 (2005).

Rijssenbeek J T, Saito T, Malo S, Azuma M, Takano M, Poeppelmeier K R: Effect of Explicit Cationic Size and Valence Constraints on the Phase Stability of 1:2 B-Site-Ordered Perovskite Ruthenates, *J. Am. Chem. Soc*., **127**, 675-681 (2005).

Belik A A, Azuma M, Saito T, Shimakawa Y, Takano M: Crystallographic Features and Tetragonal Phase Stability of $PbVO_3$, a New Member of $PbTiO_3$ Family, *Chem. Mater*., **17**, 269-273 (2005).

Belik A A, Azuma M, Matsuo A, Kindo K, Takano M: Low-Dimensional Ferromagnetic Properties of $SrCuV_2O_7$ and $BaCuV_2O_7$, *Inorg. Chem*., **44**, 3762-3766 (2005).

Belik A A, Matsuo A, Azuma M, Kindo K, Takano M: Long-Range Magnetic Ordering of S=1/2 Linear Trimers in $A_3Cu_3(PO_4)_4$ (A=Ca, Sr, and Pb), *J. Solid State Chem*., **178**, 709-714 (2005).

Matsuda M, Kakurai K, Belik A A, Azuma M, Takano M, Fujita M: Magnetic Excitations from the Linear Heisenberg Antiferromagnetic Spin Trimer System $A_3Cu_3(PO_4)_4$ (A=Ca, Sr, and Pb), *Phys. Rev. B*, **71**, [144411-1]-[144411-5] (2005).

Azuma M, Takata K, Saito T, Ishiwata S, Shimakawa Y, Takano M: Designed Ferromagnetic, Ferroelectric Bi_2NiMnO_6, *J. Am. Chem. Soc*., **127**, 8889-8892 (2005).

Ishiwata S, Azuma M, Hanawa M, Moritomo Y, Ohishi Y, Kato K, Takata M, Nishibori E, Sakata M, Terasaki I, Takano M: Pressure/Temperature/Substitution-Induced Melting of A-Site Charge Disproportionation in $Bi_{1-x}La_xNiO_3$ ($0 \leq x \leq 0.5$), *Phys. Rev. B*, **72**, [045104-1]-[045104-7] (2005).

Kan D, Terashima T, Shimakawa Y, Takano M: Fabrication and *I-V* Characteristics of *p-n* Junctions Composed of High-T_c Superconductors and La-Doped $SrTiO_3$, *Thin Solid Films*, **486**, 71-74 (2005).

Yamamoto S, Takano M, Shimakawa Y: Synthesis of Submicron-Sized, Monodisperse Spherical V_2O_5 Particles, *Mater. Res. Soc. Symp. Proc*., **879E**, [Z7.14.1]-[Z7.14.6] (2005).

Inagaki Y, Narumi Y, Kindo K, Kikuchi H, Kamikawa T, Kunimoto T, Okubo S, Ohta H, Saito T, Azuma M, Takano M, Nojiri H, Kaburagi M, Tonegawa T: Ferro-Antiferromagnetic Delta-Chain System Studied by High Field Magnetization Measurements, *J. Phys. Soc. Jpn*., **74**, 2831-2835 (2005).

Shimakawa Y, Azuma M, Takata K, Hashisaka M, Kan D, Masuno A, Sakai M, Terashima T, Mibu K, Takano M: New Ferromagnetic Ferroelectric Bi_2NiMnO_6 Compound with Double-Perovskite Structure, *Proceedings of the 12th US-Japan Seminar on Dielectric and Piezoelectric Ceramics, Nov. 6-9, 2005, Annapolis, USA*, 203-206 (2005).

Belik A A, Izumi F, Azuma M, Kamiyama T, Oikawa K, Pokholok K V, Lazoryak B I, Takano M: Redox Reactions in Strontium Iron Phosphates: Synthesis, Structures, and Characterization of $Sr_9Fe(PO_4)_7$ and $Sr_9FeD(PO_4)_7$, *Chem. Mater*., **17**, 5455-5464 (2005).

Belik A A, Azuma M, Matsuo A, Whangbo M-H, Koo H-J, Kikuchi J, Kaji T, Okubo S, Ohta H, Kindo K, Takano M: Investigation of the Crystal Structure and the Structural and Magnetic Properties of $SrCu_2(PO_4)_2$, *Inorg. Chem*., **44**, 6632-6640 (2005).

Qiu Y, Broholm C, Ishiwata S, Azuma M, Takano M, Bewley R, Buyers W J L: Spin-Trimer Antiferromagnetism in $La_4Cu_3MoO_{12}$, *Phys. Rev. B*, **71**, [214439-1]-[214439-8] (2005).

Okubo S, Taketani A, Ohta H, Kunimoto T, Inagaki Y, Saito T, Azuma M, Takano M, Kikuchi H: High Field ESR Measurements of S=1/2 Diamond Chain Substance $Cu_3(CO_3)_2(OH)_2$ at the Magenetization Plateau Region, *Progress of Theoretical Physics Supplement*, **No.159**, 11-16 (2005).

Shiraki K, Yoshida M, Okubo S, Ohta H, Belik A A, Azuma M, Takano M: High Field ESR Measurements of $MCuP_2O_7$ (M=Sr, Pb), *Progress of Theoretical Physics Supplement*, **No.159**, 168-172 (2005).

Belik A A, Azuma M, Takano M: Magnetic Properties of Isostructural $BaCoP_2O_7$, $BaNiP_2O_7$ and $BaCuP_2O_7$ Studied with dc and ac Magnetization and Specific Heat, *Inorg. Chem*., **44**, 7523-7529 (2005).

Wadati H, Takizawa M, Tran T T, Tanaka K, Mizokawa T, Fujimori A, Chikamatsu A, Kumigashira H, Oshima M, Ishiwata S, Azuma M, Takano M: Valence Changes Associated with the Metal-Insulator Transition in $Bi_{1-x}La_xNiO_3$, *Phys. Rev. B*, **72**, [155103-1]-[155103-5] (2005).

Kan D, Terashima T, Kanda R, Masuno A, Tanaka K, Chu S, Kan H, Ishizumi A, Kanemitsu Y, Shimakawa Y, Takano M: Blue-Light Emission at Room Temperature from Ar^+-Irradicated $SrTiO_3$, *Nature Materials*, **4**, 816-819 (2005).

[Others]

Azuma M: Solid–Liquid Equilibria and Eutectic Mixtures, *Kagakubinran Kisohen, Maruzen*, [II-194]-[II-198] (2004) (in Japanese).

DIVISION OF MATERIALS CHEMISTRY
— Chemistry of Polymer Materials —

Kubo K, Goto A, Sato K, Kwak Y, Fukuda T: Kinetic Study on Reversible Addition-Fragmentation Chain Transfer (RAFT) Process for Block and Random Copolymerizations of Styrene and Methyl Methacrylate, *Polymer* , **46**, 9762-9768 (2005).

Kwak Y, Goto A, Fukuda T, Yamago S, Ray B: Mechanism and Kinetics of Organostibine-Mediated Living Radical Polymerization of Styrene, *Z. Chem. Phys*., **219**, 283-294 (2005).

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**, 2137-2142 (2005).

Yoshikawa C, Goto A, Tsujii Y, Fukuda T, Yamamoto K, Kishida A: Fabrication of High-Density Polymer Brush on Polymer Substrate by Surface-Initiated Living Radical Polymerization, *Macromolecules*, **38**, 4604-4610 (2005).

Koh K, Sugiyama S, Morinaga T, Ohno K, Tsujii Y, Fukuda T, Yamahiro M, Iijima T, Oikawa H, Watanabe K, Miyashita T: Precision Synthesis of a Fluorinated Polyhedral Oligomeric Silsesquioxane-Terminated Polymer and Surface Characterization of Its Blend Film with Poly(methyl mehtacrylate), *Macromolecules*, **38**, 1264-1270 (2005).

Norisuye T, Morinaga T, Tang-Cong-Miyata Q, Goto A, Fukuda T, Shibayama M: Comparison of the Gelation Dynamics for Polystyrenes Prepared by Conventional and Living Radical Polymerizations: A Time-Resolved Dynamic Light Scattering Study, *Polymer*, **46**, 1982-1994 (2005).

Sakakiyama T, Ohkita H, Ohoka M, Ito S, Tsujii Y, Fukuda T: Fabrication and Electrochemical Properties of High-Density Graft Films with Ferrocene Moieties on ITO Substrates, *Chem. Lett*., **34**, 1366-1367 (2005).

Barner-Kowollik C, Buback M, Egorov M, Fukuda T, Goto A, Olja O F, Russell G T, Vana P, Yamada B, Zetterlund P B: Critically Evaluated Termination Rate Coefficients for Free-Radical Polymerization: Experimental Methods, *Prog. Polym. Sci*., **30**, 605-643 (2005).

Chung H -J, Ohno K, Fukuda T, Composto R J: Self-Regulated Structures in Nanocomposites by Directed Nanoparticle Assembly, *Nano Lett*., **5**, 1878-1882 (2005).

Ito S, Kuno J, Yamashita K, Ohoka M, Ohkita H, Tsujii Y, Fukuda T: Photofunctional Ultrathin Films Prepared by High-Density Graft Polymerization, *Trans. Mater. Res. Soc. Jpn*, **30**, 687-690 (2005).

Ifuku S, Tsujii Y, Kamitakahara H, Takano T, Nakatsubo F: Preparation and Characterization of Redox Cellulose Langmuir-Blodgett Films Containing a Ferrocene Derivative, *J. Polym. Sci. Part A: Polym. Chem*., **43**, 5023-5031 (2005).

Ifuku S, Kamitakahara H, Takano T, Tsujii Y, Nakatsubo F: Preparation and Characterization of 6-*O*-(4-Stearyloxytrityl)cellulose Acetate Langmuir-Blodgett Films, *Cellulose*, **12**, 361-369 (2005).

Ifuku S, Nakai S, Kamitakahara H, Takano T, Tsujii Y, Nakatsubo F: Preparation and Characterization of Monolayer and Multilayer Langmuir-Blodgett Films of a Series of 6-*O*-Alkylcelluloses, *Biomacromolecules*, **6**, 2067-2073 (2005).

McNamee C E, Tsujii Y, Matsumoto M: Physicochemical Characterization of an Anatase TiO_2 Surface and the Adsorption of a Nonionic Surfactant: An Atomic Force Microscopy Study, *Langmuir*, **21**, 11283-11288 (2005).

Arita T, Beuermann S, Buback M, Vana P: RAFT Polymerization of Methyl Acrylate in Carbon Dioxide, *Macromol. Mater. Eng*., **209**, 283-293 (2005).

Arita T, Buback M, Vana P: Cumyl Dithiobenzoate Mediated RAFT Polymerization of Styrene at High Temperatures, *Macromolecules*, **38**, 7935-7943 (2005).

Fukuda T: Growing Polymer Brushes from Solid Surfaces, *Koubunshi*, **54**, 483-488 (2005) (in Japanese).

Fukuda T: Copolymerization, *Cyclopedia of Polymers, Soc. Polym. Sci. Jpn. Ed., Asakura* (2005) (in Japanese).

Tsujii Y, Fukuda T: Graft Polymerization from Inorganic Surfaces, *Nano-Composite Materials-Nanocomposites of Metals, Ceramics, and Polymers- Inoue A. Ed., Frontier Publishers, Tokyo*, 261-266 (2005) (in Japanese).

Tsujii Y: Studies on Precise Surface Modification by Living Radical Polymerization, *Sen-I Gakkaishi*, **61**, 260-263 (2005) (in Japanese).

Goto A, Kwak Y, Fukuda T: Rate Retardation in Reversible Addition-Fragmentation Chain Transfer (RAFT)-Based Living Radical Polymerization: Precision Analysis in Styrene/Dithiobenzoate System, *Ann. Rep. Res. Inst. Chem. Fib. (Kasen-Kouenshu)*, **62**, 67-72 (2005) (in Japanese).

— Chemistry of Polymeric Functionality Materials —

Poompradub S, Kohjiya S, Ikeda Y: Natural Rubber/In Situ Silica Nanocomposite of a High Silica Content, *Chem. Lett*., **34**, 672-673 (2005).

Steinhart M, Murano S, Schaper A K, Ogawa T, Tsuji M, Goesele U, Weder C, Wendorff J H: Morphology of Polymer/Liquid-Crystal Nanotubes: Influence of Confinement, *Adv. Funct. Mater*., **15**, 1656-1664 (2005).

Poompradub S, Tosaka M, Kohjiya S, Ikeda Y, Toki S, Sics I, Hsiao B S: Mechanism of Strain-Induced Crystallization in Filled and Unfilled Natural Rubber Vulcanizates, *J. Appl. Phys*., **97**, [103529-1]-[103529-9] (2005).

Bedia E L, Kasai Y, Ikeda Y, Kohjiya S: Effect of Mount Pinatubo Volcanic Ash on the Mechanical Properties of Styrene-Butadiene Rubber Vulcanizates, *J. Appl. Polym. Sci*., **95**, 68-73 (2005).

Kojima M, Tosaka M, Ikeda Y, Kohjiya S: Devulcanization of Carbon Black Filled Natural Rubber by Using Supercritical Carbon Dioxide, *J. Appl. Polym. Sci*., **95**, 137-143 (2005).

Hirano K, Suzuki K, Nakano K, Tosaka M: Phase Separation Structure in the Polymer Blend of Fluorocarbon Elastomer and Hydrogenated Nitrile Rubber, *J. Appl. Polym. Sci*., **95**, 149-156 (2005).

Terashita F, Takagi S, Kohjiya S, Naito Y: Airtight Butyl Rubber under High Pressures in the Storage Tank of CARS-G/T System Power Plant, *J. Appl. Polym. Sci*., **95**, 173-177 (2005).

Senoo K, Endo K: Synthesis and Characterization of Syndiotactic Polystyrene-Polyisoprene-Syndiotactic Polystyrene ABA Type Triblock Copolymers, *J. Macromol. Sci., Part A*, **A42**, 463-470 (2005).

Kohjiya S, Katoh A, Shimanuki J, Hasegawa T, Ikeda Y: Nano-Structural Observation of Carbon Black Dispersion in Natural Rubber Matrix by Three-Dimensional Transmission Electron Microscopy, *J. Mater. Sci*., **40**, 2553-2555 (2005).

Saikrasun S, Bualek-Limcharoen S, Kohjiya S, Urayama K: Anisotropic Mechanical Properties of Thermoplastic Elastomers In Situ Reinforced with Thermotropic Liquid-Crystalline Polymer Fibers Revealed by Biaxial Deformations, *J. Polym. Sci.: Part B: Polym. Phys*., **43**, 135-144 (2005).

Kojima M, Tosaka M, Funami E, Nitta K, Ohshima M, Kohjiya S: Phase Behavior of Crosslinked Polyisoprene Rubber and Supercritical Carbon Dioxide, *J. Supercrit. Fluids*, **35**, 175-181 (2005).

Kohjiya S, Katoh A: Visualization of Nanostructure in Soft Materials by 3D-TEM, *Kobunshi Ronbunshu*, **62**, 467-475 (2005) (in Japanese).

Toki S, Sics I, Hsiao B S, Tosaka M, Poompradub S, Ikeda Y, Kohjiya S: Probing the Nature of Strain-Induced Crystallization in Polyisoprene Rubber by Combined Thermomechanical and In Situ X-ray Diffraction Techniques, *Macromolecules*, **38**, 7064-7073 (2005).

Tosaka M, Danev R, Nagayama K: Application of Phase Contrast Transmission Microscopic Methods to Polymer Materials, *Macromolecules*, **38**, 7884-7886 (2005).

Yoshioka T, Tsuji M, Kawahara Y, Kikutani T, Kohjiya S: Internal Fine Structures in the High-Speed-Spun Fibers of Poly(Ethylene 2,6-Naphthalene Dicarboxylate), *Polymer*, **46**, 1886-1892/5429-5432 (2005).

Kojima M, Kohjiya S, Ikeda Y: Role of Supercritical Carbon Dioxide for Selective Impregnation of Decrosslinking Reagent into Isoprene Rubber Vulcanizate, *Polymer*, **46**, 2016-2019 (2005).

Kohjiya S, Katoh A, Shimanuki J, Hasegawa T, Ikeda Y: Three-Dimensional Nano-Structure of In Situ Silica in Natural Rubber as Revealed by 3D-TEM/Electron Tomography, *Polymer*, **46**, 4440-4446 (2005).

Yoshioka T, Tsuji M, Kawahara Y, Kohjiya S, Manabe N, Yokota Y: Morphological Study by TEM on Uniaxially Oriented Thin Films of PBT, *Polymer*, **46**, 4987-4990 (2005).

Senoo K, Matsuda S, Kohjiya S: Preparation of Physical Gel Consisting of Syndiotactic Polystyrene and Poly(Ethylene Glycol), *Polymer*, **46**, 7819-7822 (2005).

[Others]

Kohjiya S: *Butsurigaku Jiten (Dictionary of Physics), 3rd Edition, Ed by Editorial Committee of Butsurigaku Jiten, Baifukan, Tokyo (Partial Contribution)* (2005) (in Japanese).

Kohjiya S: Nano-Technology and Soft-Matter, *Nano-Technology and Soft Matter, Ed by The Society of Rubber Industry, Japan, Posty Corp, Tokyo,* **Chap 1**, 1-7 (2005) (in Japanese).

Kohjiya S, Senoo K, Ikeda Y: Polymer Solid Electrolytes for Lithium-Ion Conduction, *Solid State Ionics for Batteries, Ed by Minami T, Tatsumisago M, Wakihara M, Iwakura C, Kohjiya S, Tanaka I, Springer Verlag, Tokyo,* **Chap 6**, 187-223 (2005).

Kohjiya S, Tosaka M, Furutani M, Poompradub S, Ikeda Y: Smart In-Situ Nano-Composite: Strain-Induced Crystallization of Natural Rubber, *Ann. Rep. Res. Inst. Chem. Fiber, Jpn*., **62**, 53-65 (2005) (in Japanese).

Kohjiya S, Tsuji M, Tosaka M: *Kobunshi Jiten (Dictionary of Polymer Science), 3rd Edition, Ed by the Society of Polymer Science, Japan, Asakura Shoten, Tokyo (Partial Contribution)* (2005) (in Japanese).

Senoo K: Structural Control of Soft Materials, *Kobunshi*, **54**, 142 (2005) (in Japanese).

Tosaka M, Murakami S, Poompradub S, Kohjiya S, Ikeda Y, Toki S, Sics I, Hsiao B S: Orientation and Crystallization of Natural Rubber Network as Revealed by WAXD Using Synchrotron Radiation, *National Synchrotron Light Source 2004 Activity Report*, [2-92]-[2-93] (2005).

Tsuji M, Yoshioka T: Kaisetsu (Diffraction), *Jikken Kagaku Koza 5th Edition, Vol 26 Kobunshi Kagaku, Section 3.4.1, Ed by Chem. Soc. Japan, Maruzen, Tokyo*, 302-315 (2005) (in Japanese).

Furutani M, Tosaka M, Kohjiya S, Ikeda Y: Effects of Non-Rubber Components on Strain-Induced Crystallization of Natural Rubber Vulcanizates, Especially of Stearic Acid, *Adhesion and Adhesives*, **49**, 202-207 (2005) (in Japanese).

Katoh A, Ikeda Y, Kohjiya S: Three-Dimensional Observation of Nano Filler-Filled Natural Rubber Vulcanizates by 3D-Transmission Electron Microscopy (3D-TEM), *The Journal of the Society of Rubber Industry, Japan*, **78**, 180-186 (2005) (in Japanese).

— Inorganic Photonics Materials —

Miyabe D, Takahashi M, Tokuda Y, Yoko T, Uchino T: Structure and Formation Mechanism of Six-Fold Coordinated Silicon in Phosphosilicate Glasses, *Phys. Rev. B*, **71**, [172202-1]-[172202-4] (2005).

Mizuno M, Takahashi M, Takaishi T, Yoko T: Leaching of Lead and Connectivity of Plumbate Networks in Lead Silicate Glasses, *J. Am. Ceram. Soc*, **88**, 2908-2912 (2005).

Yoshida Y, Fujii J, Muroi K, Otsuka A, Saito G, Takahashi M, Yoko T: Highly Conducting Ionic Liquids Based on 1-Ethyl-3-methylimidazolium Cation, *Synth. Metals*, **153**, 421-424 (2005).

Yoshida Y, Otsuka A, Saito G, Natsume S, Nishibori E, Takata M, Sakata M, Takahashi M, Yoko T: Conducting and Magnetic Properties of 1-Ethyl-3-methylimidazolium (EMI) Salts Containing Paramagnetic Irons: Liquids $[EMI][M^{III}Cl_4]$ (M = Fe and $Fe_{0.5}Ga_{0.5}$) and Solid $[EMI]_2[Fe^{II}Cl_4]$, *Bull. Chem. Soc. Jpn*., **78**, 1921-1928 (2005).

Innocenzi P, Kidchob T, Yoko T: Hybrid Organic-Inorganic Sol-Gel Materials Based on Epoxy-Amine Systems, *J.Sol-Gel Sci. & Tech*., **35**, 225-235 (2005).

Dorjpalam E, Takahashi M, Tokuda Y, Yoko T: Controlling Carrier Density and Its Effect on I-V Characteristics of The Anatase-TiO_2 Thin Films Prepared by A Sputter Deposition Method, *Thin Solid Films*, **483**, 147-151 (2005).

Takaishi T, Takahashi M, Jin J, Uchino T, Yoko T: Structural Study on $PbO\text{-}SiO_2$ Glasses by X-Ray and Neutron Diffraction and Si-29 MAS NMR Measurements, *J. Am. Ceram. Soc*., **88**, 1591-1596 (2005).

Mori R, Takahashi M, Yoko T: Gel-Melting Method for Preparation of Organically Modified Siloxane Low-Melting Glasses, *J. Mater. Res*., **20**, 121-127 (2005).

Masai H, Takahashi M, Tokuda Y, Yoko T: Gel-Melting Method for Preparation of Organically Modified Siloxane Low-Melting Glasses, *J. Mater. Res*., **20**, 1234-1241 (2005).

Masai H, Takahashi M, Tokuda Y, Yoko T: Enhancement of Polycondensation Reaction by Diethyl Ether-Aqueous NaOH Immiscible Two Phase Liquid Treatment of Phenyl-Modified Polysiloxane Glass, *J. Ceram. Soc. Jpn*., **113**, 259-262 (2005).

— Magnetic Materials —

Yamaguchi A, Nasu S, Tanigawa H, Ono T, Miyake K, Mibu K, Shinjo T: Effect of Joule Heating in Current-driven Domain Wall Motion, *Appl. Phys. Lett*., **86**, [012511-1]-[012511-3] (2005).

Miyake K, Shigeto K, Yokoyama Y, Ono T, Mibu K, Shinjo T: Exchange Biasing of a Néel Wall in the Nanocontact between NiFe Wires, *J. Appl. Phys*., **97**, [014309-1]-[014309-6] (2005).

Himeno A, Okuno T, Ono T, Mibu K, Nasu S, Shinjo T: Temperature Dependence of Depinning Fields in Submicron Magnetic Wires with an Artificial Neck, *J. Magn. Magn. Mater*., **286**, 167-170 (2005).

Miura K, Ono T, Nasu S, Okuno T, Mibu K, Shinjo T: Electrical Spin Injection in $Ni_{81}Fe_{19}$/Al/$Ni_{81}Fe_{19}$ with Double Tunnel Junctions, *J. Magn. Magn. Mater*., **286**, 142-145 (2005).

Nakamura N, Ogi H, Hirao M, Ono T: Elastic Constants and Magnetic Anisotropy of Co/Pt Superlattice Thin Films, *Appl. Phys. Lett*., **86**, [111918-1]-[111918-3] (2005).

Nakamura N, Ogi H, Ono T, Hirao M, Nishiyama M: Elastic Constants and Magnetic Anisotropy in Co/Pt Superlattice: Resonance Ultrasound Spectroscopy Method, Jpn. *J. Appl. Phys*., **44**, 4427-4430 (2005).

Nakamura N, Ogi H, Hirao M, Ono T: Determination of Anisotropic Elastic Constants of Superlattice Thin Films by Resonant-ultrasound Spectroscopy, *J. Appl. Phys*., **97**, [013532-1]-[013532-6] (2005).

Himeno A, Okuno T, Kasai S, Ono T, Nasu S, Mibu K, Shinjo T: Propagation of a Magnetic Domain Wall in Magnetic Wires with Asymmetric Notches, *J. Appl. Phys*., **97**, [066101-1]-[066101-3] (2005).

Nakamura N, Ogi H, Ono T, Hirao M: Elastic Constants for Co/Pt Nano-multilayers by Resonance Ultrasound Spectroscopy, *Review of Quantitative Nondestructive Evaluation*, **24**, 1145-1150 (2005).

Yamamoto S, Morimoto Y, Ono T, Takano M: Magnetically Superior and Easy to Handle $L1_0$-FePt Nanocrystals, *Appl. Phys. Lett*., **87**, [032503-1]-[032503-3] (2005).

Sato M, Aikawa H, Kobayashi K, Katsumoto S, Iye Y: Observation of the Fano-Kondo Anti-Resonance in a Quantum Wire with a Side-Coupled Quantum Dot, *Phys. Rev. Lett*., **95**, [1066801-1]-[1066801-4] (2005).

Saitoh E, Kasai S, Miyajima H, Yamaoka T: Electron Coherence and Magnetic Structure in a Nanostructured Ferromagnetic Ring, *J. App. Phys*., **97**, [10J709-1]-[10J709-3] (2005).

DIVISION OF BIOCHEMISTRY
— Biofunctional Design-Chemistry —

Futaki S, Masui Y, Nakase I, Sugiura Y, Nakamura T, Kogure K, Harashima H: Unique Features of a pH-sensitive Fusogenic Peptide that Improves the Transfection Efficiency of Cationic Liposomes, *J. Gene Med*, **7**, 1450-1458 (2005).

Noguchi H, Matsumoto S, Okitsu T, Iwanaga Y, Yonekawa Y, Nagata H, Matsushita M, Wei F Y, Matsui H, Minami K, Seino S, Masui Y, Futaki S, Tanaka K: PDX-1 Protein Is Internalized by Lipid Raft-dependent Macropinocytosis, *Cell Transplantation*, **14**, 637-645 (2005).

Yamada Y, Shinohara Y, Kakudo T, Chaki S, Futaki S, Kamiya H, Harashima H: Mitochondrial Delivery of Mastoparan with Transferrin Liposomes Equipped with a pH-sensitive Fusogenic Peptide for Selective Cancer Therapy, *Int. J. Pharm*., **13**, 1-7 (2005).

Okamura E, Ninomiya K, Futaki S, Nagai Y, Kimura T, Wakai C, Matubayasi N, Sugiura Y, Nakahara M: Real-time In-cell ^{19}F NMR Study on Uptake of Fluorescent and Nonfluorescent ^{19}F-Octaarginines into Human Jurkat Cells, *Chem. Lett*., **34**, 1064-1065 (2005).

Mudhakir D, Akita H, Khalil I A, Futaki S, Harashima H: Pharmacokinetic Analysis of the Tissue Distribution of Octaarginine Modified Liposomes in Mice Drug Metab., *Pharmacokinet*., **20**, 275-281 (2005).

Moriguchi R, Kogure K , Akita H, Futaki S, Miyagishi M, Taira K, Harashima H: A Multifunctional Envelope-type Nano Device for Novel Gene Delivery of siRNA Plasmids, *Int. J. Pharm*., **301**, 277-285 (2005).

Noguchi H, Nakai Y, Matsumoto S, Kawaguchi M, Ueda M, Okitsu T, Iwanaga Y, Yonekawa Y, Nagata H, Minami K, Seino S, Masui Y, Futaki S, Tanaka K: Cell Permeable Peptide of JNK Inhibitor Prevents Islet Apoptosis Immediately after Isolation and Improves Islet Graft Function, *Am. J. Transplant*., **5**, 1848-1855 (2005).

Futaki S: Membrane-permeable Arginine-rich Peptides and the Translocation Mechanisms, *Adv. Drug Deliv. Rev*., **57**, 547-558 (2005).

Perret F, Nishihara M, Takeuchi T, Futaki S, Lazar A N, Coleman A, Sakai N, Matile S: Anionic Fullerenes, Calixarenes, Coronenes, and Pyrenesas Activators of Oligo/Polyarginines in Model Membranes and Live Cells, *J. Am. Chem. Soc*., **127**, 1114-1115 (2005).

Nishihara M, Perret F, Takeuchi T, Futaki S, Lazar A N, Coleman A, Sakai N, Matile S: Arginine Magic with New Counterions up the Sleeve, *Org. Biomol. Chem*., **3**, 1659-1669 (2005).

Imanishi M, Yan W, Morisaki T, Sugiura Y: An Artificial Six-zinc Finger Peptide with Polyarginine Linker: Selective Binding to the Discontinuous DNA Sequences, *Biochemical and Biophysical Research Communications*, **333**, 137-173 (2005).

Hirata T, Nomura W, Imanishi M, Sugiura Y: Effects of Linking 15-zinc Finger Domains on DNA Binding Specificity and Multiple DNA Binding Modes, *Bioorg Med Chem Lett*, **15**, 2197-2201 (2005).

Nakatsukasa T, Shiraishi Y, Negi S, Imanishi M, Futaki S, Sugiura Y: Site-specific DNA Cleavage by Artificial Zinc Finger-type Nuclease with Cerium-binding Peptide, *Biochemical and Biophysical Research Communications*, **330**, 247-252 (2005).

Shiraishi Y, Imanishi M, Morisaki T, Sugiura Y: Swapping of the Beta-hairpin Region between Sp1 and GLI Zinc Fingers: Significant Role of the Beta-hairpin Region in DNA Binding Properties of C2H2-type Zinc Finger Peptides, *Biochemistry*, **44**, 2523-2528 (2005).

Sakai N, Takeuchi T, Futaki S, Matile S: Direct Observation of Anion-Mediated Translocation of Fluorescent Oligoarginine Carriers Into and Across Bulk Liquid and Anionic Bilayer Membranes, *ChemBioChem*., **6**, 114-122 (2005).

Futaki S, Kiwada T, Sugiura Y: Control of Peptide Structure and Recognition by Fe(III)-induced Helix Destabilization, *J. Am. Chem. Soc*., **126**, 15762-15769 (2004).

Futaki S, Nakase I, Suzuki T, Nameki D, Kodama E: RNase S Complex Bearing Arginine-rich Peptide and Anti-HIV Activity, *J. Mol. Recogn*., **18**, 169-174 (2004).

— Chemistry of Molecular Biocatalysts —

Ueno K, Yoneyama H, Saito S, Mizutani M, Sakata K, Hirai N, Todoroki Y: A Lead Compound for the Development of ABA 8'-Hydroxylase Inhibitors, *Bioorg. Med. Chem. Lett*., **53**, 5226-5229 (2005).

Ueno K, Araki Y, Hirai N, Saito S, Mizutani M, Sakata K, Todoroki Y: Differences between the Structural Requirements for ABA 8'-Hydroxylase Inhibition and for ABA Activity, *Bioorg. Med. Chem*., **13**, 3359-3370 (2005).

Sawai Y, Moon J-H, Sakata K, Watanabe N: Effects of Structure on Radical-scavenging Abilities and Antioxidative Activities of Tea Polyphenols: NMR Analytical Approach Using 1,1-Diphenyl-2-picrylhydorazyl Radicals, *J. Agric. Food Chem*., **53**, 3598-3614 (2005).

Kato M, Uno T, Hiratake J, Sakata K: α-Glucopranoimidazolines as Intemediate Analogue Inhibitors of Family 20 β-*N*-Aetylglycosaminidases, *Bioorg. Med. Chem*., **13**, 1563-1571 (2005).

Fujii R, Nakagawa Y, Hiratake J, Sogabe A, Sakata K: Directed Evolution of *Pseudomonas aeruginosa* Lipase for Improved Amide-hydrolyzing Activity, *Protein Engineering, Design and Selection*, **18**, 93-101 (2005).

Hiratake J: Enzyme Inhibitors as Chemical Tools to Study Enzyme Catalysis: Rational Design, Synthesis, and Applications, *The Chemical Record*, **5**, 209-228 (2005).

Fujita K, Oura F, Nagamine N, Katayama T, Hiratake J, Sakata K, Kumagai H, Yamamoto K: Identification and Molecular Cloning of a Novel Glycoside Hydrolase Family of Core 1 Type *O*-Glycan-specific endo-α-*N*-Acetylgalactosaminidase from *Bifidobacterium longum, J. Biol. Chem*., **280**, 37415-37422 (2005).

Nakanishi T, Nakatsu T, Matsuoka M, Sakata K, Kato H: Crystal Structures of Pyruvate Phosphate Dikinase from Maize Revealed an Alternative Conformation in the Swiveling-domain Mortion, *Biochemistry*, **44**, 1136-1144 (2005).

Kinoshita T, Cho J-Y, Mizutani M, Shimizu B, Tsai H-T, Chen Y-L, Lin M-L, Sakata K: Gene Expression Profiling in the Manufacturing Process of "Oriental Beauty", *Proceedings of 2004 International Conference on O-Cha (tea) Culture and Science*, 161-164 (2005).

Ogura M, Terada I, Shirai F, Tokoro K, Chen K-R, Chen C-L, Lin M-L, Shimnizu B, Kinoshita T, Sakata K: Tracing Aroma Characteristics Changes during Porecessing of the Famous Formosa Oolong Tea "Oriental Beauty", *Proceedings of 2004 International Conference on O-Cha (tea) Culture and Science*, 240-242 (2005).

Sawai Y, Yamaguchi Y, Mizukami Y, Sakata K, Watanabe N: Comparison of Radical-Scavenging Abilities and Influence of Conjugated Double Bond on Antioxidative Activities of Tea Polyphenols, *Proceedings of 2004 International Conference on O-Cha (tea) Culture and Science*, 256-257 (2005).

Cho J-Y, Shimizu B, Kinoshita T, Mizutani M, Chen K-R, Chen C-L, Sakata K: Chemical Profiling in the Manufacturing Process of "Oriental Beauty", *Proceedings of 2004 International Conference on O-Cha (tea) Culture and Science*, 260-262 (2005).

Mizutani M: Diversity of Cytochromes P450 and Chemical Evolution in Plants, *Regulation of Plant Growth and Development*, **40**, 67-82 (2005).

Mizutani M, Saito S: Enhancement of Drought Tolerance by P450 Inhibitors in Plants, *Kagaku to Seibutsu*, **43**, 628-630 (2005).

— Molecular Biology —

[Others]

Oka A, Ohashi Y, Aoyama T: Contribution of Phospholipase D to Morphogenesis of Plant Epidermal Cells, *Genes & Genetic Systems*, **79**, 377-377 (2004).

Tsuge T, Dohmae N, Wei N, Oka A: Novel Regulation of COP9 Signalosome (CSN): a Master Regulator of Signal Transduction in Plant Morphogenesis, *Plant Cell Physiol*., **46**, S241-S241 (2005).

Taniguchi M, Aoyama T, Oka A: Screening for Genes Directly Regulated by ARR1, *Plant Cell Physiol*., **46**, S38- S38 (2005).

Tsuge T, Oka A: Will the Research in Plant Light Signaling Contribute to the Cure of Cancer? –The Frontier Research of COP9 Signalosome, *Kagaku*, **60**, 72-73 (2005) (in Japanese).

Aoyama T: Experimental System for Protein Function Inducible with Mammalian Steroid Hormones, *A Series of Shokubutu Saibou Kougaku: Experimental Protocol with Model Plants (eds: Shimamoto K, Okada K, Tabata S)*, **21**, 226-229 (2005) (in Japanese).

— Chemical Biology —

[Others]

Uesugi M: Small Molecules That Control Gene Expression, *Seikagaku*, **77(9)**, 1177-1180 (2005) (in Japanese).

Kawazoe Y, Uesugi M: Trends in Chemical Libraries for Chemical Genetics, *Tanpakushitsu Kakusan Koso*, **50(9)**, 1043-1048 (2005) (in Japanese).

Tanaka S, Takehashi M, Iida S, Kitajima T, Kamanaka Y, Stedeford T, Banasik M, Ueda K: Mitochondrial Impairment Induced by Poly(ADP-ribose) Polymerase-1 Activation in Cortical Neurons after Oxygen-Glucose Deprivation, *J. Neurochem.,* **95**, 179-190 (2005).

Strosznajder RP, Jesko H, Banasik M, Tanaka S: Effects of p53 Inhibitor on Survival and Death of Cells Subjected to Oxidative Stress, *J. Physiol. Pharmacol.*, **56**, 215-221 (2005).

DIVISION OF ENVIRONMENTAL CHEMISTRY
— Molecular Materials Chemistry —

Kaji H, Kusaka Y, Onoyama G, Horii F: Relation between Light-Emitting Properties and Different Isomers in Polymorphs of Tris(8-hydroquinoline) Aluminum(III) (Alq_3) Analyzed by Solid-State ^{27}Al NMR and DFT Calculations, *Jap. J. Appl. Phys*., **44**, 3706-3711 (2005).

Kaji H, Yamada T, Tsukamoto N, Horii F: A Combined Experimental and Theoretical Study of the Conformation of N,N'-Diphenyl-N,N'-Di(m-tolyl)benzidine (TPD) Using Solid-State ^{15}N NMR and DFT Calculations, *Chem. Phys. Lett*., **401**, 246-253 (2005).

Kimura F, Kimura T, Tamura M, Hirai A, Ikuno M, Horii F: Magnetic Alignment of the Chiral Nematic Phase of a Cellulose Microfibril Suspension, *Langmuir*, **21**, 2034-2037 (2005).

[Others]

Horii F, Hirai A, Suzuki F: Disordered Structure of Native Cellulose and Its Production Origin, *Cellulose Commun*., **12**, 179-183 (2005) (in Japanese).

Horii F: Cellulose – New Viewpoints for the Most Abundant Organic Resources on the Earth, *Environ. Preserv*., **No.20**, 38-46 (2005) (in Japanese).

Horii F, Hirai A, Suzuki F: Hierarchical Structure of Bacterial Cellulose – Sturucture of Sub-Elementary Fibrils and Their Structural Evolution, *Meet. Rep. Poval Commit*., **No.127**, 21-28 (2005) (in Japanese).

Horii F: Magnetic Relaxation; Spin-Lattice Relaxation; Spin-Spin Relaxation; Correlation Function; Correlation Time, *Polymer Dictionary*, **3rd Ed**, 253, 311, 311, 341, 341 (2005) (in Japanese).

— Hydrospheric Environment Analytical Chemistry —

Gamo T, Masuda H, Yamanaka T, Okamura K, Ishibashi J, Nakayama E, Obata H, Shitashima K, Nishio Y, Hasumoto H, Watanabe M, Mitsuzawa K, Seama N, Tsunogai U, Kouzuma F, Sano Y: Discovery of a New Hydrothermal Venting Site in the Southernmost Mariana Arc: Al-Rich Hydrotermal Plumes and White Smoker Activity Associated with Biogenic Methane, *Geochem. J*., **38**, 527-534 (2004).

Ezoe M, Ishita T, Kinugasa M, Lai X, Norisuye K, Sohrin Y: Distributions of Dissolved and Acid-Dissolvable Bioactive Trace Metals in the North Pacific Ocean, *Geochem. J*., **38**, 535-550 (2004).

Okamura K, Hatanaka H, Kimoto H, Suzuki M, Sohrin Y, Nakayama E, Gamo T, Ishibashi J: Development of an *In-situ* Manganese Analyzer Using Micro-Diaphragm Pumps and Its Application to Time-Series Observations in a Hydrothermal Field at the Suiyo Seamount, *Geochem. J*., **38**, 635-642 (2004).

Kinugasa M, Ishita T, Sohrin Y, Okamura K,Takeda S, Nishioka J, Tsuda A: Dynamics of Trace Metals during the Subarctic Pacific Iron Experiment for Ecosystem Dynamics Study (SEEDS 2001), *Prog. Oceanogr*., **64**, 129-147 (2005).

Umetani S, Matsumoto H, Kurahashi K: Synergistic Extraction of Metal Ions with Novel Bidentate Neutral Ligands, *Proceedings of ISEC2005*, 188-193 (2005).

Minami T, Sohrin Y, Ueda J: Determination of Chromium, Copper and Lead in River Water by Graphite-Furnace Atomic Absorption Spectrometry after Coprecipitation with Terbium Hydroxide, *Anal. Sci*., **21**, 1519-1521 (2005).

[Others]

Sohrin Y, Okamura K: *Advanced Analytical Methods (Umezawa Y, Sawada T, Terabe S, eds.)*, 861-865 (2004) (in Japanese).

Sohrin Y, Ezoe M, Kinugasa M, Lai X, Norisuye K: Distribution of Bioactive Trace Metals in the Pacific, *Kaiyo Monthly*, **39**, 54-60 (2005) (in Japanese).

Fujinaga T, Sohrin Y, Isshiki K, eds.: *Chemistry of the Ocean and Lakes–Studying with Trace Elements*, (2005) (in Japanese).

Ishibashi J, Nakamura K, Okamura K, Shitashima K, Toki T, Tsunogai U: Development of Sampling Devices and Monitoring System to Study the Geochemical Environment within Active Hydrothermal Fluid, *Umino Kenkyu*, **14**, 251-266 (2005) (in Japanese).

Tsunogai U, Nakagawa F, Okamura K: Geochemical Studies on the Microbial Activities within the Suiyo Seamount Hydrothermal Plume, Izu-Bonin Arc, *Umino Kenkyu*, **14**, 279-296 (2005) (in Japanese).

— Solution and Interface Chemistry —

Nagai Y, Morooka S, Matubayasi N, Nakahara M: Mechanism and Kinetics of Aldehyde Reaction in Supercritical Water: Noncatalytic Disproportionation, Condensation, and Decarbonylation, *J. Phys. Chem. A*, **108**, 11635-11643 (2004).

Okamura E, Wakai C, Matubayasi N, Sugiura Y, Nakahara M: Limited Slowdown of Endocrine-Disruptor Diffusion in Confined Fluid Lipid Membranes, *Phys. Rev. Lett*., **93**, [248101-1]-[248101-4] (2004).

Matubayasi N, Nakahara M: Hydrothermal Reactions of Small Compounds: Free-energy Analysis of Equilibrium, *J. Chem. Phys*., **122**, [074509-1]-[074509-12] (2005).

Nagai Y, Matubayasi N, Nakahara M: Mechanisms and Kinetics of Noncatalytic Ether Reaction in Supercritical Water. 1. Proton-Transferred Fragmentation of Diethyl Ether to Acetaldehyde in Composition to Hydrolysis, *J. Phys. Chem. A*, **109**, 3550-3557 (2005).

Nagai Y, Matubayasi N, Nakahara M: Mechanisms and Kinetics of Noncatalytic Ether Reaction in Supercritical Water. 2. Proton-Transferred Fragmentation of Dimethyl Ether to Acetaldehyde in Composition to Hydrolysis, *J. Phys. Chem. A*, **109**, 3558-3564 (2005).

Morooka S, Wakai C, Matubayasi N, Nakahara M: Hydrothermal Carbon-Carbon Bond Formation and Disproportionations of C1 Aldehydes: Formaldehyde and Formic Acids, *J. Phys. Chem. A*, **109**, 6610-6619 (2005).

Okamura E, Ninomiya K, Futaki S, Nagai Y, Kimura T, Wakai C, Matubayasi N, Sugiura Y, Nakahara M: Real-Time In-Cell ^{19}F-NMR Study on Uptake of Fluorescent and Nonfluorescent ^{19}F-Octaarginines into Human Jurkat Cells, *Chem. Lett*., **34**, 1064-1065 (2005).

Yoshida K, Wakai C, Matubayasi N, Nakahara M: A New High-Temperature Multinuclear Magnetic Resonance Probe and the Self-Diffusion of Light and Heavy Water in Sub- and Supercritical Conditions, *J. Chem. Phys*., **122**, [164506-1]-[164506-10] (2005).

Wakai C, Oleinikova A, Ott M, Weingärtner H: How Polar Are Ionic Liquids? Determination of the Static Dielectric Constant of an Imidazolium-based Ionic Liquid by Microwave Dielectric Spectroscopy, *J. Phys. Chem. B*, **109**, 17028-17030 (2005).

Nakahara M: Hitoshi Ohtaki-Autobiography, *J. Mol. Liq*., **119**, 5-6 (2005).

Matubayasi N, Nakahara M: An Approach to the Solvation Free Energy in Terms of the Distributions Functions of the Solute-Solvent Interaction Energy, *J. Mol. Liq*., **119**, 23-29 (2005).

Yamaguchi T, Matubayasi N, Nakahara M: Nuclear Magnetic Resonance and Molecular Dynamics Simulation Study on the Reorientational Relaxation of Solutes in Supercritical Methanol, *J. Mol. Liq*., **119**, 119-123 (2005).

Nakahara M: Structure, Dynamics, and Reactions in Supercritical Water Studied by NMR and Computer Simulation, *Water, Steam, and Aqueous Solutions for Electric Power Edited by M. Nakahara, N. Matubayasi, M. Ueno, K. Yasuoka, and K. Watanabe*, 12-23 (2005).

Matubayasi N, Nakahara M: Hydrothermal Reactions of Formic Acid: Free-Energy Analysis of Equilibrium, *Water, Steam, and Aqueous Solutions for Electric Power Edited by M. Nakahara, N. Matubayasi, M. Ueno, K. Yasuoka, and K. Watanabe*, 313-318 (2005).

[Others]

Nakahara M: Supercritical Fluid Reactions in Relation to Energy Problem, *News Letter, Society High-Temp. High-Pressure Technol*., **32**, 1-1 (2004) (in Japanese).

Nakahara M: Roles of Supercritical-Fluid Reactions for 21st Century Energy Problems -Synthesis of Dimethyl Ether and Hydrogen-, *Jasco Report*, **8**, 30-34 (2004) (in Japanese).

Matubayasi N, Nakahara M: Statistical Thermodynamics of Hydration and Supercritical and Hot Water Chemistry for Energy and Environmental Issues, *CHEMISTRY TODAY*, **410**, 40-44 (2005) (in Japanese).

Nakahara M: NMR Studies on Water and Aqueous Solution in Supercritical and High-Pressure Conditions, *The Review of High Pressure Science and Technology*, **15**, 224-237 (2005) (in Japanese).

Nakahara M: Chemical Evolution on the Primitive Earth Learned from Studies on Supercritical Water Reactions, *Transactions of The Research Institute of Oceanochemistry*, **18**, 83-88 (2005) (in Japanese).

Okamura E, Nakahara M: Static and Dynamic NMR Studies of Anesthetics in Membranes, *Anesth. Resus*., **41**, 21-22 (2005) (in Japanese).

Nakahara M: Mesurements of Fluid Properties at High-Pressures, *The Fifth Series of Experimantal Chemistry Vol.6 Chemical Thermodynamics and High-Pressure Science Edited by Chemical Sciety of Japan*, **Chapter11.4**, 460-461 (2005) (in Japanese).

Nakahara M, et al.: *Chronological Scientific Table 2005 Edited by National Astronomical Observatory*, **78**, 484-491,496-499 (2005) (in Japanese).

— Molecular Microbial Science —

Yoshimune K, Galkin A, Kulakova L, Yoshimura T, Esaki N: Cold-active DnaK of an Antarctic Psychrotroph *Shewanella* sp. Ac10 Supporting the Growth of *dnaK*-Null Mutant of *Escherichia coli* at Cold Temperatures, *Extremophiles*, **9**, 145-150 (2005).

Yoshimune K, Galkin A, Kulakova L, Yoshimura T, Esaki N: DnaK from *Vibrio proteolyticus*: Complementation of a *dnaK*-Null Mutant of *Escherichia coli* and the Role of Its ATPase Domain, *J. Biosci. Bioeng*., **99**, 136-142 (2005).

Yoshimune K, Esaki N, Moriguchi M: Site-directed Mutagenesis Alters DnaK-dependent Folding Process, *Biochem. Biophys. Res. Commun*., **326**, 74-78 (2005).

Yamamoto H, Mitsuhashi K, Kimoto N, Kobayashi Y, Esaki N: Robust NADH-regenerator: Improved α-Haloketone-resistant Formate Dehydrogenase, *Appl. Microbiol. Biotechnol*., **67**, 33-39 (2005).

Muramatsu H, Mihara H, Kakutani R, Yasuda M, Ueda M, Kurihara T, Esaki N: The Putative Malate/Lactate Dehydrogenase from *Pseudomonas putida* Is an NADPH-dependent Δ^1-Piperideine-2-Carboxylate/Δ^1-Pyrroline-2-Carboxylate Reductase Involved in the Catabolism of D-Lysine and D-Proline, *J. Biol. Chem*., **280**, 5329-5335 (2005).

Muramatsu H, Mihara H, Goto M, Miyahara I, Hirotsu K, Kurihara T, Esaki N: A New Family of NAD(P)H-dependent Oxidoreductases Distinct from Conventional Rossmann-Fold Proteins, *J. Biosci. Bioeng*., **99**, 541-547 (2005).

Mihara H, Muramatsu H, Kakutani R, Yasuda M, Ueda M, Kurihara T, Esaki N: *N*-Methyl-L-amino Acid Dehydrogenase from *Pseudomonas putida*. A Novel Member of an Unusual NAD(P)-dependent Oxidoreductase Superfamily, *FEBS J*., **272**, 1117-1123 (2005).

Kurata A, Kurihara T, Kamachi H, Esaki N: 2-Haloacrylate Reductase, A Novel Enzyme of the Medium Chain Dehydrogenase/reductase Superfamily That Catalyzes the Reduction of a Carbon-carbon Double Bond of Unsaturated Organohalogen Compounds, *J. Biol. Chem*., **280**, 20286-20291 (2005).

Igarashi M, Maruoka N, Kato S, Mihara H, Kurihara T, Esaki N: Characterization of Slr0077 of *Synechocystis* sp. PCC6803, a Homolog of Chloroplastic Cysteine Desulfurase of Higher Plants, *Trace Nutrients Research*, **21**, 51-58 (2004).

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
— Polymer Materials Science —

Kanaya T, Kakurai K, Tsukushi I, Inoue R, Watanabe H, Nishi M, Nakajima K, Takemura K, Furuya H: Thermal Neutron Spin-echo Studies on Dynamics of a Glass-forming Polymer in a High Q Range, *J. Phys. Soc. Jpn*., **74**, 3236-3240 (2005).

Kaji K, Nishida K, Kanaya T, Matsuba G, Konishi T, Imai M: Spinodal Crystallization of Polymers: Crystallization from the Unstable Melt, *Adv. Polym. Sci*., **191**, 187-240 (2005).

Haefele A, Heck B, Hippler T, Kawai T, Kohn P, Strobl G: Crystallization of Poly(ethylene-co-octene): II - Melt Memory Effects on First Order Kinetics, *Eur. Phys. J. E*., **16**, 217-224 (2005).

Sharma L, Nishida K, Kanaya T: FT-IR Study of the Morphological Interactions in PHB/PAZO Blends and Their Dependence on Solvent Variation, *Polymers & Polymer Composites*, **13**, 681-686 (2005).

Haefele A, Heck B, Kawai T, Kohn P, Strobl G: Crystallization of a Poly(ethylene-co-octene): I - A Precursor Structure and Two Competing Mechanisms, *Eur. Phys. J. E*., **16**, 207-216 (2005).

Konishi T, Nishida K, Kanaya T, Kaji K: Effect of Isotacticity on Formation of Mesomorphic Phase of Isotactic Polypropylene, *Macromolecules*, **38**, 8749-8754 (2005).

Sharma L, Nishida K, Kanaya T: The Effect of Solvent on the Miscibility of Blends of Poly 1-[4-(3-carboxy-4-hydroxyphenylazo)benzene sulphonamido-1,2-ethanediyl, sodium salt] (PAZO) and Polyhydroxybutyrate, (PHB), *Polymers & Polymer Composites*, **13**, 443-452 (2005).

Inoue R, Kanaya T, Nishida K, Tsukushi I, Shibata K: Inelastic Neutron Scattering Study of Low Energy Excitations in Polymer Thin Films, *Phys. Rev. Lett*., **95**, [056102-1]-[056102-4] (2005).

Kanaya T, Monkenbusch M, Watanabe H, Nagao M, Richter D: Dynamics of Deuterated Polystyrene-Protonated Butadiene Diblock Copolymer Micelles by Neutron Spin Echo, *J. Chem. Phys*., **122**, 144905-144913 (2005).

Nakamura K, Shikata T, Takahashi N, Kanaya T: Highly Extended Conformation of Polyelectrolytes Incorporated into Hybrid Threadlike Micelles Studied by Small Angle Neutron Scattering, *J. Am. Chem. Soc*., **127**, 4570-4571 (2005).

Kanaya T, Miyazaki T, Inoue R, Nishida K: Thermal Expansion and Contraction of Polymer Thin Films, *Phys. Status. Solidi (b)*, **242**, 595-606 (2005).

Kanaya T, Takahashi N, Nishida K, Seto H, Nagao M, Takeda T: Neutron Spin-Echo Studies on Dynamic and Static Fluctuations in Two Types of Poly(vinyl alcohol) Gels, *Phys. Rev. E*., **71**, [011801-1]-[011801-7] (2005).

Fukushima H, Ogino Y, Matsuba G, Nishida K, Kanaya T: Crystallization of Polyethylene Under Shear Flow as Studied by Time Resolved Depolarized Light Scattering. Effects of Shear Rate and Shear Strain, *Polymer*, **46**, 1878-1885 (2005).

Takahashi N, Kanaya T, Nishida K, Kaji K: Small-Angle Neutron Scattering Study of Poly(vinyl alcohol) Gels during Melting Process, *J. Appl. Polym. Sci*., **47**, 157-160 (2005).

[Others]

Nishida K: Inversion of Interaction in Polyelectrolyte Solution, *SEN-I GAKKAISHI*, **61**, 14-18 (2005) (in Japanese).

Kanaya T: University and Collaborative Research, *SEN-I GAKKAISHI*, **61**, 119 (2005) (in Japanese).

Kanaya T: Polymer Crystallization under Shear Flow, *Seikei-Kakou*, **17**, 479-483 (2005) (in Japanese).

Kanaya T, Miyazaki T, Inoue R, Nishida K: Glass Tansition of Polymer Thin Films, *Kasen Kouenshu*, **62**, 39-44 (2005) (in Japanese).

Kanaya T, Ogino Y, Fukushima H, Matsuba G, Nishida K: Polymer Crystallization under Shear Flow, *Structure and Dynamics in Macromolecular Systems with Specific Interactions*, 49-56 (2005).

Kanaya T: Neutron Scattering, *Experimental Lecture of Chemistry*, **26**, 331-341 (2005) (in Japanese).

Kanaya T: Structure of Polymer Crystal, *Experimental Lecture of Chemistry*, **26**, 379-386 (2005) (in Japanese).

— Molecular Rheology —

Yoshida T, Kanaoka S, Watanabe H, Aoshima S: Stimuli-Responsive Reversible Physical Networks. II. Design and Properties of Homogeneous Physical Networks Consisting of Periodic Copolymers Synthesized by Living Cationic Polymerization, *J. Polym. Sci. A: Polym. Chem*., **43**, 2712-2722 (2005).

Watanabe H, Matsumiya Y, Inoue T: Dielectric and Viscoelastic Study of Entanglement Dynamics: A Review of Recent Findings, *Macromolecular Symposia*, **228**, 51-70 (2005).

Watanabe H, Matsumiya Y, Ishida S, Takigawa T, Yamamoto T, Vlassopoulos D, Roovers J: Nonlinear Rheology of Multiarm Star Chains, *Macromolecules*, **38**, 7404-7415 (2005).

Horigome M, Yada M, Koike J, Watanabe H: Viscoelastic Behavior and Its Mechanisms of Aqueous Suspensions of Resin Particles, *J. Jap. Soc. Col. Mat*., **78**, 299-303 (2005).

Kujawa P, Watanabe H, Tanaka F, Winnik F M: Amphiphilic Telechelic Poly(N-isopropylacrylamide) in Water: From Micelles to Gels, *Euro. Phys. J. E*., **17**, 129-137 (2005).

Watanabe H: Viscosity, *Nishinari, Okoshi, Kouyama, Yamamoto Eds.," Food Texture Handbook", Science Forum, Tokyo, Chapter 1, Section 2*, 163-168 (2005).

Watanabe H, Matsumiya Y: Rheology of Diblock Copolymer Micellar Dispersions Having Soft Cores, *Macromolecules*, **38**, 3808-3819 (2005).

Watanabe H, Inoue T: Conformational Dynamics of Rouse Chains during Creep/recovery Processes: a Review, *J. Phys. Condensed Matter*, **17**, R607-R636 (2005).

Matsuda Y, Sato T, Oishi Y, Watanabe H: Association of Polybutadiene Living Anions in Cyclohexane, *J. Polym. Sci. B: Polym. Phys*., **43**, 1401-1407 (2005).

Inoue T, Shikata T: Nonlinear Rheology of Thread-like Micellar Aquerous Solution, *Oleo Sci*., **5**, 327-334 (2005) (in Japanese).

Kanaya T, Monkenbusch M, Watanabe H, Nagao M, Richter D: Dynamics of Deuterated Polystyene-Protonated Butadiene Diblock Copolymer Micelles by Neutron Spin Echo, *J. Chem. Phys*., **122**, [144905-1]-[144905-9] (2005).

Tian P, Uhrig D, Mays J W, Watanabe H, Kilbey II S M: Role of Branching on the Structure of Polymer Brushes Formed From Comb Copolymers, *Macromolecules*, **38**, 2524-2529 (2005).

Inoue T, Inoue Y, Watanabe H: Nonlinear Rheology of CTAB/NaSal Aqueous Solutions: Finite Extensibility of a Network of Wormlike Micelles, *Langmuir*, **21**, 1201-1208 (2005).

Urayama K, Okada S, Nosaka S, Watanabe H, Takigawa T: Kinetics of Shrinkage of Polymer Gels Induced by Ultracentrifugal Fields, *J. Chem. Phys*., **122**, [024906-1]-[024906-6] (2005).

Yaoita T, Isaki T, Masubuchi Y, Watanabe H, Ianniruberto G, Greco F, Marrucci G: Highly Entangled Polymer Primitive Chain Network Simulations Based on Dynamic Tube Dilation, *J. Chem. Phys*., **121**, 12650-12654 (2004).

Matsumiya Y, Watanabe H: Nonlinear Relaxation Behavior of Diblock Copolymer Micellar Dispersions: Effects of Corona-Matrix and Corona-Corona Entanglements, *Macromolecules*, **37**, 9861-9871 (2004).

Matsuno K, Inoue T, Watanabe H: Birefringence and Viscoelasticity of Graft Copolymer, *J. Soc. Material. Sci*., **53**, 1263-1266 (2004).

— Molecular Aggregation Analysis —

Sato N, Harada Y, Terashima T, Kanda R, Takano M: Study of Thin Films of Carrier-Doped Strontium Titanate with Emphasis on Their Interfaces with Organic Thin Films, *Appl. Surf. Sci*., **244**, 588-592 (2005).

Murdey R, Liang S J S, Stuckless J T: An Atom-Transparent Photon Block for Metal-Atom Deposition from High-Temperature Ovens, *Rev. Sci. Instrum*., **76**, [023911-1]-[023911-6] (2005).

Murdey R J, Salaneck W R: Charge Injection Barrier Heights Across Multilayer Organic Thin Films, *Jpn. J. Appl. Phys*., **44**, 3751-3756 (2005).

Katoh K, Akutagawa T, Nakamura T: Molecular Design, Synthesis and Functions of Amphiphilic bis-TTF Annulated Macrocycles Forming Molecular Assembly Nanostructures, *J. Synth. Org. Chem., Jpn*., **63**, 960-969 (2005) (in Japanese).

Asami K: Simulation of Dielectric Relaxation in Periodic Binary Systems of Complex Geometry, *J. Colloid Interface Sci*., **292**, 228-235 (2005).

Asami K: Dielectric Relaxation in a Water-Oil-Triton X-100 Microemulsion Near Phase Inversion, *Langmuir*, **21**, 9032-9037 (2005).

Sekine K, Watanabe Y, Hara S, Asami K: Boundary-Element Calculations for Dielectric Behavior of Doublet-Shaped Cells, *Biochim. Biophys. Acta*, **1721**, 130-138 (2005).

— Supramolecular Biology —

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).

Aoyagi K, Sugaya T, Umeda M, Yamamoto S, Terakawa S, Takahashi M: The Activation of Exocytic Sites by the Formation of Phosphatidylinositol-4,5-bisphosphate Microdomains at Syntaxin Clusters, *J. Biol. Chem*., **280**, 2089-2104 (2005).

Nishibori A, Kusaka J, Hara J, Umeda M, Matsumoto K: Phosphatidylethanolamine Domains and Localization of Phospholipid Synthase in *Bacillus subtilis* Membranes, *J. Bacteriol*., **187**, 2163-2174 (2005).

Kobayashi H, Umeda M: A Novel Protein Lysenin, *Comp. Physiol. Biochem*., **22** (2005) (in Japanese).

Takeuchi K, Umeda M: Membrane Lipid Dynamics and Biological Thermosensor: An Approach for Molecular Lipid Biology Using Behavioral Genetics of Drosophila, *Jikken-igaku*, **23**, 961-967 (2005) (in Japanese).

Kato U, Inadome H, Umeda M: Transbilayer Movement of Lipids: Asymmetric Lipid Distribution and Flip-flop, *New Applications of Liposome for Approaches to Artificial Cells. Ed. by Akiyoshi K, Tujii K, NTS Inc*., 190-203 (2005) (in Japanese).

Inadome H, Noda Y, Adachi H, Yoda K: Immunoisolaton of the Yeast Golgi Subcompartments and Characterization of a Novel Membrane Protein, Svp26, Discovered in the Sed5-containing Compartments, *Mol. Cell. Biol*., **25**, 7696-7710 (2005).

Shishioh N, Hong Y, Ohishi K, Ashida H, Maeda Y, Kinoshita T: GPI7 is the Second Partner of PIG-F and Involved in Modification of Glycosylphosphatidylinositol, *J. Biol. Chem*., **280**, 9728-9734 (2005).

Ashida H, Hong Y, Murakami Y, Shishioh N, Sugimoto N, Kim YU, Maeda Y, Kinoshita T: Mammalian PIG-X and Yeast Pbn1p are the Essential Components of Glycosylphosphatidylinositol-mannosyltransferase I, *Mol. Biol. Cell*., **16**, 1439-1448 (2005).

Kang JY, Hong Y, Ashida H, Shishioh N, Murakami Y, Morita YS, Maeda Y, Kinoshita T: PIG-V Involved in Transferring the Second Mannose in Glycosylphosphatidylinositol, *J. Biol. Chem*., **280**, 9489-9497 (2005).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE
— Particle Beam Science —

Zhong L, Nakamura S, Fukumi A, Hayashi Y, Orimo S, Nishiuchi M, Sagisaka A, Mori M, Shirai S, Iwashita Y, Noda A, Daido H: Electron Energy Spectrometer for Laser-Driven Energetic Electron Generation, *Japanese Journal of Applied Physics*, **44**, 6796-6800 (2005).

Iwashita Y: Neat Bunching Scheme with Amplitude Modulation, *Nuclear Physics B - Proceedings Supplements*, **149**, 268-270 (2005).

Ohmori C, Aoki M, Kuriyama Y, Yoshida M, Arimoto Y, Sato M, Kuno Y, Iwashita Y, Ninomiya S: Ultra-High Field Gradient RF for Bunch Rotation, *Nuclear Physics B - Proceedings Supplements*, **149**, 280-282 (2005).

Wakasugi M, Emoto T, Koseki T, Ohnishi T, Suda T, Takeda T, Yano Y, Kurita K, Shirai T, Tongu H: R&D Study of a Self-Confining Radioactive Ion Target (SCRIT) in the KSR, *Beam Science and Technology*, **9**, 3-7 (2005).

Fujimoto T, Shibuya S, Noda K, Noda A, Shirai T: Injection System for S-LSR, *Beam Science and Technology*, **9**, 8-11 (2005).

Noda A, Grieser M: Possible Scheme of Tapered Cooling by Combination of Laser Cooling and Wien Filter, *Beam Science and Technology*, **9**, 12-15 (2005).

Grieser M, Fadil H, Noda A, Shirai T: Ion Deflection in a Toroid Magnet, *Beam Science and Technology*, **9**, 16-19 (2005).

Ikegami M, Fadil H, Shirai T, Tongu H, Noda A, Ogawa H, Takeuchi T, Noda K, Shibuya S, Fujimoto T: Field Measurement of Bending Magnets for S-LSR, *Beam Science and Technology*, **9**, 20-30 (2005).

Takeuchi T, Noda K, Shibuya, S, Noda A, Shirai T, Tongu H, Fadil H, Ikegami M: Magnetic Field Measurement and Individual Characteristics of Quadrupole Magnets for S-LSR, *Beam Science and Technology*, **9**, 31-35 (2005).

Takechi T, Noda A, Fujimoto S: Magnetic Permeability of Stainless Bent Plate, *Beam Science and Technology*, **9**, 36-37 (2005).

Soda H, Takeuchi T, Ikegami M, Shirai T: Magnets Arrangement of S-LSR, *Beam Science and Technology*, **9**, 38-42 (2005).

Tongu H, Shibuya S, Shirai T, Takeuchi T, Iwashita Y, Noda A, Noda K, Fujimoto S: The Outgassing of the Vacuum Ducts for S-LSR, *Beam Science and Technology*, **9**, 43-44 (2005).

Fujimoto S, Shirai T, Noda A, Tongu H, Takeuchi T: Non-destructive Monitor Development for a Small Ion Storage Ring S-LSR, *Beam Science and Technology*, **9**, 45-47 (2005).

Nokamura S, Noda A, Iwashita Y, Shirai T, Yamazaki A, Takeuchi T, Tanabe M, Tongu H, Ikegami M, Fujimoto S, Sakabe S, Hashida M, Shimizu S: Energetic Ion Generation by Interaction between T^6-Laser and Thin Foils, *Beam Science and Technology*, **9**, 48-49 (2005).

Syresin E, Smirnov A, Noda A, Noda K, Shirai T, Fadil H: S-LSR Low Ion Energy Mode, *Beam Science and Technology*, **9**, 50-57 (2005).

[Others]

Iwashita Y, Mihara T, Kumada M, Spencer C: Field Quality and Magnetic Center Stability Achieved in a Variable Permanent Maget Quadrupole for the ILC, *Proceedings of 2005 Particle Accelerator Conference*, 1913-1915 (2005).

Fujimoto S, Shirai T, Noda A, Tongu H, Takeuchi T, Noda K: Static Beam Position Monitor for a Small Ion Storage Ring S-LSR, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 60-62 (2005) (in Japanese).

Noda A, Shirai T, Tongu H, Ikegami M, Fujimoto S, Tanabe M, Souda H, Yamada S, Noda K, Shibuya S, Iwata S, Takubo A, Takeuchi T, Fujimoto T, Fujiwara H, Fadil H, Grieser M, Meshkov I, Syresin E, Smirnov A, Sidorin A: Beam Cooling at Ion Accumulation/Cooler Ring, S-LSR, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 156-158 (2005).

Tanabe M, Noda A, Shirai T, Tongu H, Ikegami M, Souda H, Noda K, Shibuya S: Experimental Study of Dispersion Control Utilizing Both Magnetic and Electric Field, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 731-733 (2005) (in Japanese).

Tongu H, Ikegami M, Tanabe M, Shirai T, Noda A, Fujimoto S, Shibuya S, Takeuchi T, Noda K, Kanakura J, Sano M: Static Beam Position Monitor for a Small Ion StorageRing S-LSR, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 739-741 (2005) (in Japanese).

Ikegami M, Okamoto H, Shirai T, Souda H, Tanabe M, Noda A, Noda K: Beam Dynamics at Ion Storage Ring S-LSR, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 742-744 (2005) (in Japanese).

Souda H, Tanabe M, Ikegami M, Noda A: Three Dimensional Laser Cooling with Dispersion Control at S-LSR, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 808-810 (2005) (in Japanese).

Iwashita Y: Mitigation of Power Loss due to Skin Effect, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 138-140 (2005) (in Japanese).

Mihara T, Iwashita Y, Kumada M, Spencer C: Adjustment of Super-Strong Permanent Magnet Quadrupole, *Proceedings of the 2nd Annual Meeting of Particle Accelerator Society of Japan*, 227-229 (2005) (in Japanese).

— Laser Matter Interaction Science —

Sakabe S,Takahashi K, Hashida M, Shimizu S, Iida T: Elements and Their Transitions Feasible for NEET, *Atomic Data and Nuclear Data Tables*, **91**, 1-7 (2005).

Iinuma M, Matsukado K, Endo I, Hashida M, Hayashi K, Kohara A, Matsumoto F, Nakanishi Y, Sakabe S, Shimizu S, Taniuchi T, Yamamoto K, Takahashi T: Observation of Second Harmonics in Laser-Electron Scattering Using Low Energy Electron Beam, *Phys. Lett. A*, **346**, 255-260 (2005).

Hashida M, Shimizu S, Sakabe S: Nano-Ablation with Short Pulse Laser, *Rev. Laser Eng*., **33**, 514-518 (2005) (in Japanese).

Fujita M, Hashida M: Femtosecond-Laser Processing, *J. Plasma Fusion Res*., **81 suppl**., 195-201 (2005) (in Japanese).

Nishimura H, Inubushi Y, Ochiai M, Kawamura T, Fujioka S, Hashida M, Shimizu S, Sakabe S, Kodama R, Tanaka K A, Kato S, Koike F, Nakazaki S, Nagatomo H, Johzaki T, Mima K: Study of Fast Electron Transport in Hot Dense Matter Using X-ray Spectroscopy, *Plasma Phys. Control. Fusion*, **47**, B823-B831 (2005).

Shimizu S, Zhakhovskii V, Murakami M, Tanaka M, Yatsuhashi T, Okihara S, Nishihara K, Sakabe S, Izawa Y, Nakashima N: Coulomb Explosion of Hexa-Fluorobenzene Induced by an Intense Laser Field, *Chem. Phys. Lett*., **404**, 379-383 (2005).

Takagi Y, Yamada Y, Ishikawa K, Shimizu S, Sakabe S: Ultrafast Single-Shot Optical Oscilloscope Based on Time-to-Space Conversion due to Temporal and Spatial Walk-Off Effects in Nonlinear Mixing Crystal, *Jpn. J. Appl. Phys. A*, **44**, 6546-6549 (2005).

Tsukamoto M, Asuka K, Nakano H, Hashida M, Katto M, Abe N, Fujita M: Femtosecond Laser Produced Periodic Microstructures on Titanium Plate, *Adv. Appl. Plasma Scie*., **5**, 283-288 (2005).

[Others]

Setsuhara Y, Hashida M, Fujita M: Nonequilibrium Activation of Boron-Implanted Ultra-Shallow Junctions by Femtosecond-Laser Induced Phonon Excitation Process, *Proc. 4th International Conference on Silicon Epitaxy and Hetereostructures (ICSI-4) Awaji Island, Hyogo, Japan, May 23-26*, 306-307 (2005).

— Electron Microscopy and Crystal Chemistry —

Steinhart M, Murano S, Schaper A K, Ogawa T, Tsuji M, Gosele U, Weder C, Wendorff J H: Morphology of Polymer/Liquid-Crystal Nanotubes: Influence of Confinement, *Adv. Funct. Mater*., **15**, 1656-1664 (2005).

Harada M, Toshima N, Yoshida K, Isoda S: Aggregated Structure Analysis of Polymer-Protected Platinum/Ruthenium Colloidal Dispersions Using EXAFS, HRTEM, and Electron Diffraction Measurements, *J. Colloid Interface Sci*., **283**, 64-78 (2005).

Koshino M, Masunaga-Hasegawa Y, Nemoto T, Kurata H, Isoda S: Radiation Damage Analysis of 7,7,8,8,-Tetracyanoquinodimethane (TCNQ) and 2,3,5,6-Tetrafluoro-7,7,8,8-Tetracyanoquinodimethane (F_4TCNQ) by Electron Diffraction and Electron Energy Loss Spectroscopy, *Micron*, **36**, 271-279 (2005).

Yoshida K, Yaji T, Koshino M, Isoda S: Structural Analysis of Bis(1,2-benzoquinonedioximato)platinum(II) Polymorphs Formed Epitaxially on Alkali Halides, *Jpn. J. Appl. Phys*., **44**, 491-494 (2005).

Tsujimoto M, Kurata H, Nemoto T, Isoda S, Terada S, Kaji K: Influence of Nitrogen Vacancies on the N K-ELNES Spectrum of Titanium Nitride, *J. Electron Spectrosc. Relat. Phenom*., **143**, 159-165 (2005).

Hotta H, Kang S, Umeyama T, Matano Y, Yoshida K, Isoda S, Imahori H: Effects of Fullerene Substituents on Structure and Photoelectrochemical Properties of Fullerene Nanoclusters Electrophoretically Deposited on Nanostructured SnO_2 Electrodes, *J. Phys. Chem. B*, **109**, 5700-5706 (2005).

Wang F, Jiu J, Pei L, Nakagawa K, Isoda S, Adachi M: Hydrothermal Synthesis of Highly Crystallized Lepidocrocite Nanosheets of TiO_2 under Low Temperature, *Chem. Lett*., **34**, 418-419 (2005).

Minari T, Nemoto T, Isoda S: Transport Properties of Single-Grain Organic Field-Effect Transistor, *Proc. Int. Symp. on Super-Functionality Organic Devices, IPAP Conference Series 6*, 136-139 (2005).

Imahori H, Fujimoto A, Kang S, Hotta H, Yoshida K, Umeyama T, Matano Y, Isoda S: Molecular Photoelectrochemical Devices: Supramolecular Incorporation of C_{60} Molecules into Tailored Holes on Porphyrin-Modified Gold Nanoclusters, *Adv. Mater*., **17**, 1727-1730 (2005).

Wang F, Jiu J, Pei L, Nakagawa K, Isoda S, Adachi M: Reconstruction of Lepidocrocite Nanosheets into Anatase TiO_2 by Rolling in Low Temperature, *Chem. Lett*., **34**, 1238-1239 (2005).

— Structural Molecular Biology —

Mima J, Hayashida M, Fujii T, Narita Y, Hayashi R, Ueda M, Hata Y: Structure of the Carboxypeptidase Y Inhibitor I^c in Complex with the Cognate Proteinase Reveals a Novel Mode of the Proteinase-Protein Inhibitor Interaction, *J. Mol. Biol*., **346**, 1323-1334 (2005).

Shigeoka N, Oohashi H, Tochio T, Ito Y, Mukoyama T, Vlaicu A M, Yoshikawa H, Fukushima S: [K+L] Double-electron Transition in Fe, *Physica Scripta*, **T115**, 1084-1087 (2005).

Shigeoka N, Oohashi H, Tochio T, Ito Y, Mukoyama T, Vlaicu A M, Yoshikawa H, Fukushima S: Analysis of $K\alpha$" Spectra in X-ray Emission Spectroscopy, *Physica Scripta*, **T115**, 1080-1083 (2005).

Fukao S, Nakanishi Y, Ito Y, Yoshikado S: Excitation of X-ray Using Polarized $LiNbO_3$ Single Crystal, *Key Engineering Materials*, **301**, 205-208 (2005).

Uno M, Oritsuka M, Ito Y, Yoshikado S: Synthesis and Evaluation of $Pb_{1-x}Sn_xF_2$ by a Mechanical Milling Method, *Solid State Ionics*, **176**, 2493-2498 (2005).

[Others]

Hata Y, Hayashida M, Fujii T, Mima J, Hayashi R, Ueda M: Structure and Inhibition Mode of Protein I^c in Complex with Carboxypeptidase Y, *Acta Cryst*., **A61 (Supplement)**, C190 (2005).

Horiguchi D, Yokoi K, Mizota H, Sakakura S, Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa H, Fukushima S, Yamaoka H, Shoji T: Potential of a High-resolution Anti-parallel Two-crystal Spectrometer at BL15XU in SPring-8, *The 24th International Conference on Photonic, Electronic and Atomic Collisions*, 684 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa M, Fukushima S: Behavior of $L\beta_2$ Visible Satellites in Gold Using Thresold Excitation, *The 24th International Conference on Photonic, Electronic and Atomic Collisions*, 33 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa M, Fukushima S: On Satellites Hidden by Diagram Lne in Gold, *The 24th International Conference on Photonic, Electronic and Atomic Collisions*, 32 (2005).

Ito Y, Tochio T, Oohashi H, Vlaicu A M: $K\alpha_{1,2}$ Emission Spectra in Transition Elements, *The 24th International Conference on Photonic, Electronic and Atomic Collisions*, 31 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa M, Fukushima S: Appearance of $_{78}$Pt $L\beta_{15}$ Emission Spectra by Threshold Excitation in SPring-8, *The 24th International Conference on Photonic, Electronic and Atomic Collisions*, 28 (2005).

Mizota H, Oohashi H, Ito Y, Tochio T, Yoshikado S: X-ray Emission from $LiTaO_3$ Induced by Thermal Changes and Structure Analysis, *The 20th International Conference of X-ray and Inner-shell Processes*, 245 (2005).

Vlaicu A M, Oohashi H, Tochio T, Ito Y, Horiguchi D, Yokoi K, Yoshikawa H, Takekawa S, Kitamura K: Resonant X-ray Emission Spectroscopy Study of $LiTaO_3$ Compounds, *The 20th International Conference of X-ray and Inner-shell Processes*, 235 (2005).

Vlaicu A M, Oohashi H, Tochio T, Ito Y, Horiguchi D, Yokoi K, Yoshikawa H, Nakazawa H, Fukushima S, Yamaoka H, Shoji T: Anti-parallel Crystal Spectrometer at BL15XU in SPring-8, *The 20th International Conference of X-ray and Inner-shell Processes*, 193 (2005).

Yokoi K, Oohashi H, Ito Y, Tochio T, Shoji T: $K\alpha_{3,4}$ Satellites in Na–P Elements, *The 20th International Conference of X-ray and Inner-shell Processes*, 169 (2005).

Vlaicu A M, Tochio T, Oohashi H, Ito Y, Mukoyama T, Fukushima S, Yoshikawa H: The $L_3M_{4,5}N_5$ Satellite Transition for Z=73-79, *The 20th International Conference of X-ray and Inner-shell Processes*, 168 (2005).

Sakakura S, Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Ikenaga E, Kobayashi K: Natural Widths and Coster-Kronig Transitions of Lx-ray Spectra in Elements between Pd and Sb, *The 20th International Conference of X-ray and Inner-shell Processes*, 164 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa H, Fukushima S: On Satellites Hidden by Diagram in Heavy Elements Ir, Pt, Au, *The 20th International Conference of X-ray and Inner-shell Processes*, 158 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa H, Fukushima S: Behavior of $L\beta_2$ Visible Satellites in Gold around L_1 Threshold, *The 20th International Conference of X-ray and Inner-shell Processes*, 157 (2005).

Ito Y, Tochio T, Oohashi H, Vlaicu A M: Contribution of the [1s3d] Shake Process to $K\alpha_{1,2}$ Spectra in 3d Elements, *The 20th International Conference of X-ray and Inner-shell Processes*, 156 (2005).

Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Nakazawa H, Fukushima S: The Determination of ^{78}Pt NIV - > LIII Transition Enerygy Using the Threshold Excitation Energy in SPring-8, *The 20th International Conference of X-ray and Inner-shell Processes*, 147 (2005).

Mizota H, Horiguchi D, Yokoi K, Oohashi H, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Fukushima S, Nakazawa H, Takekawa S, Kitamura K, Yoshikado S: What is the Driving Force in a Ferroelectric Material, $LiTaO_3$, *The Exciting Symposium on Excited State properties of Solids*, 15 (2005).

Yamaoka H, Ito Y, Oohashi H, Tochio T, Yokoi K, Horiguchi D, Vlaicu A M, Kawatsura K, Yamamoto K, Chainani A, Shin S, Shiga M, Wada H: High-resolution Spectroscopic Study of Atomic and Electronic Structure of Mo Compounds and Rare-earth Compounds, *SPring-8 User Experiment Report*, **14**, 92 (2005).

Fujii T, Takada Y, Uefuji H, Hashimoto H, Ito Y, Tochio T, Oohashi H, Horiguchi D, Vlaicu A M, Yoshikawa H, Fukushima S: Electric Structures of Hematite-ilmenite Solid Solution Films by Selective X-ray Emission or Absorption Spectroscopy, *SPring-8 User Experiment Report*, **14**, 93 (2005).

Oohashi H, Yokoi K, Horiguchi D, Ito Y, Tochio T, Vlaicu A M, Yoshikawa H, Fukushima S: Investigation of Valence States of Catalysts (Ag and Pt Groups) Using X-ray Fluorescence Method, *SPring-8 User Experiment Report*, **14**, 95 (2005).

Vlaicu A M, Ito Y, Yoshikawa H, Fukushima S, Yamaoka H, Okui M, Yagi N, Tochio T, Oohashi H, Sakakura S, Mizota H, Horiguchi D, Yokoi K, Shoji T, Fujimura H: Machine Evaluation of Double-crystal High-resolution X-ray Emission Spectrometer: Testing, Tuning, *SPring-8 User Experiment Report*, **14**, 254 (2005).

Vlaicu A M, Ito Y, Yoshikawa H, Fukushima S, Yamaoka H, Okui M, Yagi N, Tochio T, Oohashi H, Sakakura S, Mizota H, Horiguchi D, Yokoi K, Shoji T, Fujimura H: Investigation of Composition and Photo-induced Changes of Chemical States in $LiTaO_3$, *SPring-8 User Experiment Report*, **14**, 254 (2005).

Yamaoka H, Sugiyama H, Kubozono Y, Nouchi R, Masunari H, Vlaicu A M, Oohashi H, Sakakura S, Ito Y: High-resolution Inelastic X-ray Scattering of Metallofullerences at LIII Edge, *SPring-8 User Experiment Report*, **15**, 89 (2005).

Terashima T, Mizota H, Sakakura S, Oohashi H, Tochio T, Ito Y, Vlaicu A M, Yoshikawa H, Fukushima S: Elucidation of the Mechanism of the Luminescence in the Carrier-doped $SrTiO_3$ Fabricated by Nanoscale Technology, *SPring-8 User Experiment Report*, **15**, 90 (2005).

Horiguchi D, Ito Y, Mizota H, Oohashi H, Tochio T, Vlaicu A M, Yoshikawa H, Fukushima S, Fujimura H, Shoji T: The Property of Ba La in $BaTiO_3$, *SPring-8 User Experiment Report*, **15**, 91 (2005).

Fujii T, Takada Y, Yamashita M, Ito Y, Tochio T, Oohashi H, Vlaicu A M, Yoshikawa H, Fukushima S: Pre-edge Structures in the Ti K Edge for Various Complex Ti Oxides with the Ilmenite Structure, *SPring-8 User Experiment Report*, **15**, 91 (2005).

Vlaicu A M, Yoshikawa H, Wang Y, Mori T, Vayssieres L, Yamaoka H, Yamamoto K, Chainani A, Shin S, Okui M, Yagi N, Ito Y, Tochio T, Oohashi H, Sakakura S, Mizota H, Horiguchi D, Yokoi K: Resonant X-ray Emission Spectroscopy and Partial Fluorescence Yield XAFS Study of Rare Elements and Compounds, *SPring-8 User Experiment Report*, **15**, 255 (2005).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Organic Main Group Chemistry —

Tsuji H, Shibano Y, Takahashi T, Kumada M, Tamao K: Conformation Dependence of Photophysical Properties of σ-π Conjugation as Demonstrated by cis- and trans-1,2-Diaryl-1,2-disilacyclohexane Cyclic Systems, *Bull. Chem. Soc. Jpn*., **78**, 1334-1344 (2005).

Kawachi A, Maeda H, Tamao K: Substituent-control of Two Modes of Intramolecular Reactions of Allyloxy-silyllithiums and Propargyloxy-silyllithiums, *Bull. Chem. Soc. Jpn*., **78**, 1520-1527 (2005).

Saeki T, Son EC, Tamao K: 2-Methoxy-4-nitrobenzenediazonium Salt as a Practical Diazonium-transfer Agent for Primary Arylamines via Tautomerism of 1,3-diaryltriazenes: Deaminative Iodination and Arylation of Arylamines without Direct Diazotization, *Bull. Chem. Soc. Jpn.,* **78**, 1654-1658 (2005).

Saeki T, Takashima Y, Tamao K: Nickel- and Palladium-catalyzed Cross-coupling Reaction of Polyfluorinated Arenes and Alkenes with Grignard Reagents, *Synlett*, 1771-1774 (2005).

Yamaguchi S, Tamao K: A Key Role of Orbital Interaction in the Main Group Element-containing Pi-electron Systems, *Chem. Lett*., **34**, 2-7 (2005).

— Advanced Solid State Chemistry —

Wang D, Yu R, Chen Y, Kumada N, Kinomura N, Takano M: Photocatalysis Property of Needle-Like TiO_2 Prepared from a Novel Titanium Glycolate Precursor, *Solid State Ionics*, **172**, 101-104 (2004).

Masuno A, Terashima T, Takano M: Epitaxial Growth of Perovskite-Type $LaVO_3$ Thin Films on Various Substrates by the PLD Method, *Solid State Ionics*, **172**, 275-278 (2004).

Shen K M, Yoshida T, Lu D H, Ronning F, Armitage N P, Lee W S, Zhou X J, Damascelli A, Feng D L, Ingle N J C, Eisaki H, Kohsaka Y, Takagi H, Kakeshita T, Uchida S, Mang P K, Greven M, Onose Y, Taguchi Y, Tokura Y, Komiya S, Ando Y, Azuma M, Takano M, Fujimori A, Shen Z-X: Fully Gapped Single-Particle Excitations in Lightly Doped Cuprates, *Phys. Rev. B*, **69**, [054503-1]-[054503-5] (2004).

Masuno A, Terashima T, Shimakawa Y, Takano M: Current-Induced Electroresistive Effect in Mixed-Phase $La_{0.67}Ca_{0.33}MnO_3$ Thin Films, *Appl. Phys. Lett*., **85**, 6194-6196 (2004).

Wang D, Yu R, Xing X, Chen Y, Guo Z, Kumada N, Kinomura N, Takano M: Organic Solvent Control of Inorganic Structure: a One-Dimensional Zirconium Phosphate Inorganic Polymer, *Solid State Ionics*, **175**, 751-754 (2004).

Lebedev O I, Verbeeck J, Tendeloo G V, Hayashi N, Terashima T, Takano M: Structure and Microstructure of Epitaxial $Sr_nFe_nO_{3n-1}$ Films, *Philos. Mag*., **84**, 3825-3841 (2004).

Waku K, Katsufuji T, Kohsaka Y, Sasagawa T, Takagi H, Kishida H, Okamaoto H, Azuma M, Takano M: Charge Dynamics of $Ca_{2-x}Na_xCuO_2Cl_2$ as a Correlated Electron System with the Ideal Tetragonal Lattice, *Phys. Rev. B*, **70**, [134501-1]-[134501-8] (2004).

Azuma M, Kohsaka Y, Yamada I, Belik A A, Takagi H, Takano M: Single-Crytal Growth and New-Material Search for Oxides at High Pressures, *Oyobutsuri*, **74**, 27-31 (2005) (in Japanese).

Ninjbadgar T, Yamamoto S, Takano M: Thermal Properties of the γ-Fe_2O_3/Poly(Methyl Methacrylate) Core/Shell Nanoparticles, *Solid State Sciences*, **7**, 33-36 (2005).

Shen K M, Ronning F, Lu D H, Baumberger F, Ingle N J C, Lee W S, Meevasana W, Kohsaka Y, Azuma M, Takano M, Takagi M, Shen Z-X: Nodal Quasiparticles and Antinodal Charge Ordering in $Ca_{2-x}Na_xCuO_2Cl_2$, *Science*, **307**, 901-904 (2005).

Yu R, Xing X, Saito T, Azuma M, Takano M, Wang D, Chen Y, Kumada N, Kinomura N: A Novel Organically Templated Hybrid Open-Framework Manganese Phosphate-Oxalate, *Solid State Sciences*, **7**, 221-226 (2005).

Rijssenbeek J T, Saito T, Malo S, Azuma M, Takano M, Poeppelmeier K R: Effect of Explicit Cationic Size and Valence Constraints on the Phase Stability of 1:2 B-Site-Ordered Perovskite Ruthenates, *J. Am. Chem. Soc*., **127**, 675-681 (2005).

Belik A A, Azuma M, Saito T, Shimakawa Y, Takano M: Crystallographic Features and Tetragonal Phase Stability of $PbVO_3$, a New Member of $PbTiO_3$ Family, *Chem. Mater*., **17**, 269-273 (2005).

Belik A A, Azuma M, Matsuo A, Kindo K, Takano M: Low-Dimensional Ferromagnetic Properties of $SrCuV_2O_7$ and $BaCuV_2O_7$, *Inorg. Chem*., **44**, 3762-3766 (2005).

Belik A A, Matsuo A, Azuma M, Kindo K, Takano M: Long-Range Magnetic Ordering of S=1/2 Linear Trimers in $A_3Cu_3(PO_4)_4$ (A=Ca, Sr, and Pb), *J. Solid State Chem*., **178**, 709-714 (2005).

Matsuda M, Kakurai K, Belik A A, Azuma M, Takano M, Fujita M: Magnetic Excitations from the Linear Heisenberg Antiferromagnetic Spin Trimer System $A_3Cu_3(PO_4)_4$ (A=Ca, Sr, and Pb), *Phys. Rev. B*, **71**, [144411-1]-[144411-5] (2005).

Azuma M, Takata K, Saito T, Ishiwata S, Shimakawa Y, Takano M: Designed Ferromagnetic, Ferroelectric Bi_2NiMnO_6, *J. Am. Chem. Soc*., **127**, 8889-8892 (2005).

Ishiwata S, Wang D, Saito T and Takano M: High-Pressure Synthesis, Structure of $SrCo_6O_{11}$: Pillared Kagomé Lattice System with a 1/3 Magnetization Plateau, *Chem. Mater*., **17**, 2789-2791 (2005).

Sato N, Harada Y, Terashima T, Kanda R, Takano M: Study of Thin Films of Carrier-Doped Strontium Titanate with Emphasis on their Interfaces with Organic Thin Films, *Applied Surface Science*, **244**, 588-592 (2005).

Ishiwata S, Azuma M, Hanawa M, Moritomo Y, Ohishi Y, Kato K, Takata M, Nishibori E, Sakata M, Terasaki I, Takano M: Pressure/Temperature/Substitution-Induced Melting of A-Site Charge Disproportionation in $Bi_{1-x}La_xNiO_3$ ($0 \leq x \leq 0.5$), *Phys. Rev. B*, **72**, [045104-1]-[045104-7] (2005).

Kan D, Terashima T, Shimakawa Y, Takano M: Fabrication and *I-V* Characteristics of *p-n* Junctions Composed of High-T_c Superconductors and La-Doped $SrTiO_3$, *Thin Solid Films*, **486**, 71-74 (2005).

Yamamoto S, Takano M, Shimakawa Y: Synthesis of Submicron-Sized, Monodisperse Spherical V_2O_5 Particles, *Mater. Res. Soc. Symp. Proc*., **879E**, [Z7.14.1]-[Z7.14.6] (2005).

Yamamoto S, Morimoto Y, Ono T, Takano M: Magnetically Superior and Easy to Handle $L1_0$-FePt Nanocrystals, *Appl. Phys. Lett*., **87**, [032503-1]-[032503-3] (2005).

Inagaki Y, Narumi Y, Kindo K, Kikuchi H, Kamikawa T, Kunimoto T, Okubo S, Ohta H, Saito T, Azuma M, Takano M, Nojiri H, Kaburagi M, Tonegawa T: Ferro-Antiferromagnetic Delta-Chain System Studied by High Field Magnetization Measurements, *J. Phys. Soc. Jpn*., **74**, 2831-2835 (2005).

Kobayashi W, Ishiwata S, Terasaki I, Takano M, Grigoraviciute I, Yamauchi H, Karppinen M: Room-Temperature Ferromagnetism in $Sr_{1-x}Y_xCoO_{3-\delta}$ ($0.2 \leq x \leq 0.25$), *Phys. Rev. B*, **72**, [104408-1]-[104408-5] (2005).

Shimakawa Y, Azuma M, Takata K, Hashisaka M, Kan D, Masuno A, Sakai M, Terashima T, Mibu K, Takano M: New Ferromagnetic Ferroelectric Bi_2NiMnO_6 Compound with Double-Perovskite Structure, *Proceedings of the 12th US-Japan Seminar on Dielectric and Piezoelectric Ceramics, Nov. 6-9, 2005, Annapolis, USA*, 203-206 (2005).

Belik A A, Izumi F, Azuma M, Kamiyama T, Oikawa K, Pokholok K V, Lazoryak B I, Takano M: Redox Reactions in Strontium Iron Phosphates: Synthesis, Structures, and Characterization of $Sr_9Fe(PO_4)_7$ and $Sr_9FeD(PO_4)_7$, *Chem. Mater*., **17**, 5455-5464 (2005).

Belik A A, Azuma M, Matsuo A, Whangbo M-H, Koo H-J, Kikuchi J, Kaji T, Okubo S, Ohta H, Kindo K, Takano M: Investigation of the Crystal Structure and the Structural and Magnetic Properties of $SrCu_2(PO_4)_2$, *Inorg. Chem*., **44**, 6632-6640 (2005).

Qiu Y, Broholm C, Ishiwata S, Azuma M, Takano M, Bewley R, Buyers W J L: Spin-Trimer Antiferromagnetism in $La_4Cu_3MoO_{12}$, *Phys. Rev. B*, **71**, [214439-1]-[214439-8] (2005).

Okubo S, Taketani A, Ohta H, Kunimoto T, Inagaki Y, Saito T, Azuma M, Takano M, Kikuchi H: High Field ESR Measurements of S=1/2 Diamond Chain Substance $Cu_3(CO_3)_2(OH)_2$ at the Magenetization Plateau Region, *Progress of Theoretical Physics Supplement*, **No.159,** 11-16 (2005).

Shiraki K, Yoshida M, Okubo S, Ohta H, Belik A A, Azuma M, Takano M: High Field ESR Measurements of $MCuP_2O_7$ (M=Sr, Pb), *Progress of Theoretical Physics Supplement*, **No.159**, 168-172 (2005).

Belik A A, Azuma M, Takano M: Magnetic Properties of Isostructural $BaCoP_2O_7$, $BaNiP_2O_7$ and $BaCuP_2O_7$ Studied with dc and ac Magnetization and Specific Heat, *Inorg. Chem*., **44**, 7523-7529 (2005).

Wadati H, Takizawa M, Tran T T, Tanaka K, Mizokawa T, Fujimori A, Chikamatsu A, Kumigashira H, Oshima M, Ishiwata S, Azuma M, Takano M: Valence Changes Associated with the Metal-Insulator Transition in $Bi_{1-x}La_xNiO_3$, *Phys. Rev. B*, **72**, [155103-1]-[55103-5] (2005).

Kan D, Terashima T, Kanda R, Masuno A, Tanaka K, Chu S, Kan H, Ishizumi A, Kanemitsu Y, Shimakawa Y, Takano M: Blue-Light Emission at Room Temperature from Ar^+-Irradicated $SrTiO_3$, *Nature Materials*, **4**, 816-819 (2005).

— Organotransition Metal Chemistry —

Katayama H, Nagao M, Nishimura T, Matsui Y, Umeda K, Akamatsu K, Tsuruoka T, Nawafune H, Ozawa F: Stereocontrolled Synthesis and Optical Properties of All-cis Poly(phenylene vinylene)s (PPVs): A Method for Direct Patterning of PPVs, *J. Am. Chem. Soc*., **127**, 4350-4353 (2005).

Gajare A S, Jensen R S, Toyota K, Yoshifuji M, Ozawa F: Low-Coordinated Diphosphinidenecyclobutene Ligands: A New Entry for Stille Cross-Coupling of Aryl Bromides, *Synlett*, 144-148 (2005).

Sagawa T, Ohtsuki K, Ishiyama T, Ozawa F: Insertion of Phenylacetylene into $Pt(SnMe_3)_2(PMe_2Ph)_2$, *Organometalics*, **24**, 1470-1477 (2005).

Ozawa F, Tani T, Katayama H: C-Si Reductive Elimination from cis-Vinyl(silyl)platinum(II) Complexes, *Organometalics*, **24**, 2511-2515 (2005).

Katayama H, Yari H, Tanaka M, Ozawa F: (Z)-Selective Cross-Dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinylideneruthenium Complexes, *Chem. Commun*., 4336-4338 (2005).

Koshikawa H, Okazaki M, Matsumoto S, Ueno K, Tobita H, Ogino H: Synthesis and Structure of a Base-Stabilized Silyl(silylene)tantalum Complex, *Chem. Lett*., **34**, 1412-1413 (2005).

Suzuki E, Okazaki M, Tobita H: Reversible 1,2-Migration of Aryl Groups on Silyl Ligands: Formation and Properties of Silylenetungusten Complexes Stabilized by an External Base, *Chem. Lett*., **34**, 1026-1027 (2005).

Okazaki M, Jung K A, Tobita H: Reactivity of Phosphasilametallacyclopropane Toward Substrates with Polarized E-H Bonds (E = O, N, S, and P): Formation and Structures of Ring-Opening Products, *Organometallics*, **24**, 659-664 (2005).

Okazaki M, Jung K A, Tobita H: Regioselective Silylphosphination of Methyl Vinyl Ketone with Complexes Containing Cyclic and Linear Iron-Silicon-Phosphorus Reacting Sites, *Chem. Commun*., 912-914 (2005).

Jensen R S, Gajare A S, Toyota K, Yoshifuji M, Ozawa F: Low-Coordinated Diphosphinidene-cyclobutene Ligands: A New Entry for Palladium-Catalyzed Cyanation of Aryl Bromides, *Tetrahedron Lett*., **46**, 8645-8647 (2005).

Nagao M, Asano K, Umeda K, Katayama H, Ozawa F: Highly (Z)-Selective Hydrosilylation of Terminal Alkynes Catalyzed by a Diphosphinidenecyclobutene-coordinated Ruthenium Complex: Application to the Synthesis of (Z,Z)-Bis(2-bromoethenyl)arenes, *J. Org. Chem*., **70**, 10511-10514 (2005).

Ozawa F, Katayama H, Toyota K, Yoshifuji M: Catalytic Applications of Transition Metal Complexes Bearing sp^2-Hybridized Phosphorus Compounds, *Shokubai (Catalysts & Catalysis)*, **47**, 544-549 (2005).

Okazaki M, Takano M, Yoshimura K: Synthesis and Property of BrCCH– and BrCCBr–Coordinated Tetrairon Clusters (Organometallic Chemistry - The Next Generation - Including the 2005 Best Paper Award for a Young Investigator) , *J. Organomet. Chem*., **690**, 5318–5352 (2005).

— Photonic Elements Science —

Ishizumi A, Kanemitsu Y: Structural and Luminescence Properties of Eu-doped ZnO Nanorods Fabricated by a Microemulsion Method, *Appl. Phys. Lett*., **86**, [253106-1]-[253106-3] (2005).

Ishizumi A, Matsuda K, Saiki T, White C W, Kanemitsu Y: Photoluminescence Properties of Single Mn-doped CdS Nanocrystals Studied by Scanning Near-Field Optical Microscopy, *Appl. Phys. Lett*., **87**, [133104-1]-[133104-3] (2005).

Kan D, Terashima T, Kanda R, Masuno A, Tanaka K, Chu S, Kan H, Ishizumi A, Kanemitsu Y, Shimakawa Y, Takano M: Blue-Light Emission at Room Temperature from Ar^+-irradiated $SrTiO_3$, *Nature Materials*, **4**, 816-819 (2005).

Matsuda K, Saiki T, Nomura S, Aoyagi Y: Local Density of States Mapping of a Field-induced Quantum Dot by Near-field Photoluminescence Microscopy, *Appl. Phys. Lett*., **87**, [043112-1]-[043112-3] (2005).

Matsuda K, Kanemitsu Y, Irie K, Saiki T, Someya T, Miyauchi Y, Maruyama S: Photoluminescence Intermittency in an Individual Single-walled Carbon Nanotube at Room Temperature, *Appl. Phys. Lett*., **86**, [123116-1]-[123116-3] (2005).

Chollet M, Guerin L, Uchida N, Fukaya S, Shimoda H, Ishikawa T, Matsuda K, Hasegawa T, Ota A, Yamochi H, Saito G, Tazaki R, Adachi S, Koshihara S: Gigantic Photoresponse in 1/4-filled-Band Organic Salt, *Science*, **307**, 86-89 (2005).

Nagai T, Yamamoto A, Kanemitsu Y: Photoluminescence Dynamics of GaN under Intense Band-to-band and Exciton Resonant Excitation, *Phys. Rev. B*, **71**, [121201(R)-1]-[121201(R)-4] (2005).

Kanemitsu Y, Tomita K, Inouye H: Subpicosecond Luminescence Spectroscopy of Exciton Localization in $In_xGa_{1-x}N$ Films, *Appl. Phys. Lett*., **87**, [151120-1]-[151120-3] (2005).

Ohno Y, Shirahama T, Takeda S, Ishizumi A, Kanemitsu Y: Fe-catalytic Growth of ZnSe Nanowires on a ZnSe(001) Surface at Low Temperatures by Molecular-beam Epitaxy, *Appl. Phys. Lett*., **87**, [43105-1]-[43105-3] (2005).

Yamamoto A, Atsuta S, Kanemitsu Y: Fabrication and Photoluminescence Studies of ZnO Nanocrystals Dispersed in Glass Films, *J. Lumin.*, **112**, 169-172 (2005).

Ishizumi A, White C W, Kanemitsu Y: Photoluminescence Properties of Impurity-Doped ZnS Nanocrystals Fabricated by Sequential Ion Implantation, *Physica E*, **26**, 24-27 (2005).

Yamamoto A, Atsuta S, Kanemitsu Y: Fabrication of ZnO Nanocrystals Dispersed in Glass Films for Low-Temperature Optical Studies, *Physica E*, **26**, 96-99 (2005).

Taniguchi K, Kanemitsu Y: Development of an Apertureless Near-Field Optical Microscope for Nanoscale Optical Imaging at Low Temperatures, *Jpn. J. Appl. Phys*., **44**, 575-577 (2005).

Ishizumi A, Taguchi Y, Yamamoto A, Kanemitsu Y: Luminescence Properties of ZnO and Eu^{3+}-Doped ZnO Nanorods, *Thin Solid Films*, **486**, 50- 52 (2005).

Chollet M, Guerin L, Uchida N, Fukaya S, Ishikawa T, Koshihara S, Matsuda K, Yamochi Y, Ota A, Saito G: Ultra-Fast and Sensitive Photo-Induced Phase Switching in $(EDO\text{-}TTF)_2PF_6$, *J. Lumin*., **112**, 275-278 (2005).

BIOINFORMATICS CENTER
— Bioknowledge Systems —

Nacher J C, Yamada T, Goto S, Kanehisa M, Akutsu T: Two Complementary Representations of a Scale-free Network, *Physica A*, **349**, 349-363 (2005).

Itoh M, Goto S, Akutsu T, Kanehisa M: Fast and Accurate Database Homology Search Using Upper Bounds of Local Alignment Scores, *Bioinformatics*, **21**, 912-921 (2005).

Aoki K F, Mamitsuka H, Akutsu T, Kanehisa M: A Score Matrix to Reveal the Hidden Links in Glycans, *Bioinformatics*, **21**, 1457-1463 (2005).

Nacher J C, Ueda N, Kanehisa M, Akutsu T: Flexible Construction of Hierarchical Scale-free Networks with General Exponent, *Phys. Rev. E*., **71**, 36132 (2005).

Kucho K, Okamoto K, Tsuchiya Y, Nomura S, Nango M, Kanehisa M, Ishiura M: Global Analysis of Circadian Expression in the Cyanobacterium Synechocystis sp. Strain PCC 6803, *J. Bacteriol*., **187**, 2190-2199 (2005).

Osanai T, Kanesaki Y, Nakano T, Takahashi H, Kanehisa M, Suzuki I, Murata N, Tanaka K: Positive Regulation of Sugar Catabolic Pathways in the Cyanobacterium Synechocystis sp. PCC 6803 by the Group 2 Sigma Factor SigE, *J. Biol. Chem*., **280**, 30653-30659 (2005).

Yamanishi Y, Vert J-P, Kanehisa M: Supervised Enzyme Network Inference from the Integration of Genomic Data and Chemical Information, *Bioinformatics*, **21**, i486-i477 (2005).

Sato T, Yamanishi Y, Kanehisa M, Toh H: The Inference of Protein-protein Interactions by Co-evolutionary Analysis is Improved by Excluding the Information about the Phylogenetic Relationships, *Bioinformatics*, **21**, 3482-3489 (2005).

Hizukuri Y, Yamanishi Y, Nakamura O, Yagi F, Goto S, Kanehisa M: Extraction of Leukemia Specific Glycan Motifs in Humans by Computational Glycomics, *Carbohydr Res*., **340**, 2270-2278 (2005).

Okuda S, Kawashima S, Goto S, Kanehisa M: Conservation of Gene Co-regulation between Two Prokaryotes: Bacillus subtilis and Escherichia coli, *Genome Informatics*, **16**, 116-124 (2005).

Fujita M, Kanehisa M: Comparative Analysis of DNA-binding Proteins between Thermophilic and Mesophilic Bacteria, *Genome Informatics*, **16**, 174-181 (2005).

Yamada T, Kawashima S, Mamitsuka H, Goto S, Kanehisa M: Comprehensive Analysis and Prediction of Synthetic Lethality Using Subcellular Locations, *Genome Informatics*, **16**, 140-158 (2005).

Hashimoto K, Kawano S, Goto S, Aoki-Kinoshita KF, Kawashima M, Kanehisa M: A Global Representation of the Carbohydrate Structures: a Tool for the Analysis of Glycan, *Genome Informatics*, **16**, 214-222 (2005).

Honda W, Kawashima S, Kanehisa M: Autoimmune Diseases and Peptide Variations, *Genome Informatics*, **16**, 272-280 (2005).

Noguchi T, Ren X Q, Aoki S, Igarashi Y, Che X F, Nakajima Y, Takahashi H, Mitsuo R, Tsujikawa K, Sumizawa T, Haraguchi M, Kobayashi M, Goto S, Kanehisa M, Aikou T, Akiyama S, Furukawa T: MRP1 Mutated in the L0 Region Transports SN-38 but not Leukotriene C4 or Estradiol-17 (beta-D-glucuronate), *Biochem Pharmacol*, **70**, 1056-1065 (2005).

Tamori A, Yamanishi Y, Kawashima S, Kanehisa M, Enomoto M, Tanaka H, Kubo S, Shiomi S, Nishiguchi S: Alteration of Gene Expression in Human Hepatocellular Carcinoma with Integrated Hepatitis B Virus DNA, *Clin. Cancer. Res*., **11**, 5821-5826 (2005).

Kawano S, Hashimoto K, Miyama T, Goto S, Kanehisa M: Prediction of Glycan Structures from Gene Expression Data Based on Glycosyltransferase Reactions, *Bioinformatics*, **21**, 3976-3982 (2005).

Schwartz J M, Kanehisa M: A Quadratic Programming Approach for Decomposing Steady-state Metabolic Flux Distributions onto Elementary Modes, *Bioinformatics*, **21**, ii202-ii205 (2005).

— Biological Information Networks —

Aoki K F, Mamitsuka H, Akutsu T, Kanehisa M: A Score Matrix to Reveal the Hidden Links in Glycans, *Bioinformatics*, **21**, 1457-1463 (2005).

Ching W-K, Ng M K, Fung E S, Akutsu T: On Construction of Stochastic Genetic Networks Based on Gene Expression Sequences., *Intetnational Journal of Neural Systems*, **15**, 297-310 (2005).

Fukagawa D, Akutsu T: Performance Analysis of a Greedy Algorithm for Inferring Boolean Functions, *Information Processing Letters*, **93**, 7-12 (2005).

Hayashida M, Ueda N, Akutsu T: A Fast Method for Inferring Strengths of Protein-protein Interactions and a Hardness Result, *The IEICE Transactions*, **J88-A**, 83-90, (2005) (in Japanese).

Itoh M, Goto S, Akutsu T, Kanehisa M: Fast and Accurate Database Homology Search Using Upper Bounds of Local Alignment Scores, *Bioinformatics*, **21**, 912-921 (2005).

K.C. D, Tomita E, Suzuki J, Akutsu T: Protein Side-chain Packing Problem: A Maximum Common Edge-weight Clique Algorithmic Approach, *Journal of Bioinformatics and Computational Biology*, **3**, 103-126 (2005).

Mahé P, Ueda N, Akutsu T, Perret J-L, Vert J-P: Graph Kernels for Molecular Structure-Activity Relationship Analysis with Support Vector Machines, *Journal of Chemical Information and Modeling*, **45**, 939-951 (2005).

Matsuda S, Vert J-P, Saigo H, Ueda N, Toh H, Akutsu T: A Novel Representation of Protein Sequences for Prediction of Subcellular Location Using Support Vector Machines, *Protein Science*, **14**, 2804-2813 (2005).

Nacher J C, Yamada T, Goto S, Kanehisa M, Akutsu T: Two Complementary Representations of a Scale-free Network, *Physica A*, **349**, 349-363 (2005).

Nacher J C, Ueda N, Kanehisa M, Akutsu T: Flexible Construction of Hierarchical Scale-free Networks with General Exponent, *Physical Review E*, **71**, [036132-1]-[036132-7] (2005).

Ochiai T, Nacher J C, Akutsu T: A Stochastic Approach to Multi-Gene Expression Dynamics, *Physics Letters A*, **339**, 1-9 (2005).

Ueda N, Aoki-Kinoshita K F, Yamaguchi A, Akutsu T, Mamitsuka H: A Probabilistic Model for Mining Labeled Ordered Trees: Capturing Patterns in Carbohydrate Sugar Chains, *IEEE Transactions on Knowledge and Data Engineering*, **17**, 1051-1064 (2005).

Akutsu T, Fukagawa D: Inferring a Graph from Path Frequency, *Lecture Notes in Computer Science*, **3537**, 371-382 (2005).

Akutsu T, Fukagawa D: On Inference of a Chemical Structure from Path Frequency, *Proc. 2005 International Joint Conference of InCoB, AASBi and KSBI (BIOINFO2005)*, 96-100 (2005).

K.C. D, Tomita E, Suzuki J, Horimoto K, Akutsu T: Clique based Algorithms for Protein Threading with Profiles and Constraints, *Proc. 3rd Asia-Pacific Bioinformatics Conference (APBC 2005)*, 51-64 (2005).

K.C. D, Brown JB, Tomita E, Suzuki J, Akutsu T: Large Scale Protein Side-chain Packing Based on Maximum Edge-Weight Clique Finding Algorithm, P*roc. 2005 International Joint Conference of InCoB, AASBi and KSBI (BIOINFO2005)*, 228-233 (2005).

Meireles L M C, Akutsu T: A Gibbs Sampling Approach to Detection of Tree Motifs, *Genome Informatics*, **16**, 34-43 (2005).

Moesa H A, K. C. D, Akutsu T: Efficient Determination of Cluster Boundaries for Analysis of the Gene Expression Profile Data Using Hierarchical Clustering and Wavelet Transform, *Genome Informatics*, **16**, 132-141 (2005).

Zhang S-Q, Ng M K, Ching W-K, Akutsu T: A Linear Control Model for Gene Intervention in a Genetic Regulatory Network, *Proc. IEEE International Conference on Granular Computing (GrC 2005)*, 354-358 (2005).

[Others]

Akutsu T: Computational and Statistical Methods in Bioinformatics, *Lecture Notes in Computer Science*, **3430**, 11-33 (2005).

Akutsu T: Mathematical Models of Gene Regulatory Networks and their Inference Algorithms, *Applied Complexity Engineering*, 173-187, (2005) (in Japanese).

Akutsu T: Computational Analysis in Network Biology, *Experimental Medicine*, **23**, 609-614 (2005) (in Japanese).

— Pathway Engineering —

Mamitsuka H: Finding the Biologically Optimum Alignment of Multiple Sequences, *Artificial Intelligence in Medicine*, **35(1)**, 9-18 (2005).

Zhu S, Okuno Y, Tsujimoto G, Mamitsuka H: A Probabilistic Model for Mining Implicit "Chemical Compound - Gene" Relations from Literature, *Bioinformatics (Proceedings of the Fourth European Conference on Computational Biology (ECCB/JBI2005))*, **21, Supplement 2**, ii245-ii251 (2005).

Ueda N, Aoki-Kinoshita K F, Yamaguchi A, Akutsu T, Mamitsuka H: A Probabilistic Model for Mining Labeled Ordered Trees: Capturing Patterns in Carbohydrate Sugar Chains, *IEEE Transactions on Knowledge and Data Engineering*, **17(8)**, 1051-1064 (2005).

Mamitsuka H: Mining New Protein-Protein Interactions - Using a Hierarchical Latent-variable Model to Determine the Function of a Functionally Unknown Protein, *IEEE Engineering in Medicine and Biology Magazine*, **24(3)**, 103-108 (2005).

Mamitsuka H: Essential Latent Knowledge for Protein-Protein Interactions: Analysis by Unsupervised Learning Approach, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2(2)**, 119-130 (2005).

Mamitsuka H: Efficient Unsupervised Mining from Noisy Co-occurrence Data, *New Mathematics and Natural Computation*, **1(1)**, 173-193 (2005).

Aoki K F, Mamitsuka H, Akutsu T, Kanehisa M: A Score Matrix to Reveal the Hidden Links in Glycans, *Bioinformatics*, **21(8)**, 1457-1463 (2005).

Yamada T, Kawashima S, Mamitsuka H, Goto S, Kanehisa M: Comprehensive Analysis and Prediction of Synthetic Lethality Using Subcellular Locations, *Genome Informatics*, **16(1)**, 150-158 (2005).

Wan R, Mamitsuka H, Aoki K F: Clearning Microarray Expression Data Using Markov Random Field Based-on Profile Similarity, *Proceedings of the Twentieth ACM Symposium on Applied Computing (SAC2005)*, 206-207 (2005).

Takigawa I, Kudo M, Nakamura A: The Convex Subclass Method: Combinatorial Classifier Based on a Family of Convex Sets, *Lecture Notes in Computer Scie*nce, **3587**, 90-99 (2005).

[Others]

Cios J. K, Mamitsuka H, Nagashima T, Tadeusiewicz R: Computational Intelligence in Soving Bioinformatics Problems, *Artificial Intelligence in Medicine*, **35(1)**, 1-8 (2005).

Wan R: Book Review of 'Genomic Perl: From Bioinformatics Basics to Working Code by Rex A. Dwyer', *ACM SIGACT News*, **36(4)**, 12-Sep (2005).

Zhu S, Okuno Y, Tsujimoto G, Mamitsuka H: Mining Implict Biological Related Entities from Literature Using a Probabilistic Model, *Poster and Software Demonstrations, Sixteenth International Conference and Genome Informatics 2005 (GIW2005)*, **16**, [P006-1] - [P006-2] (2005).

Takigawa I, Mamitsuka H: Ranking Metabolic Paths with Expression Similaritiesl, *Poster and Software Demonstrations, Sixteenth International Conference and Genome Informatics 2005 (GIW2005)*, **16**, [P046-1] - [P046-2] (2005).

Wan R, Wheelock A M, Bartosiewicz M J, Mamitsuka H: Classifying Microarray Data Using Pairwise Similarity between Gene Profiles, *Poster and Software Demonstrations, Sixteenth International Conference on Genome Informatics 2005 (GIW2005)*, **16**, [P047-1] - [P047-2] (2005).

— Bioinformatics Training Unit —

Daiyasu H, Kuma K, Yokoi T, Morii H, Koga Y, Toh H: A Study of Archaeal Enzymes Involved in Polar Lipid Synthesis Linking Amino Acid Sequence Information, Genomic Contexts and Lipid Composition, *Archaea*, **1**, 399-410 (2005).

Fujiwara H, Osanai M, Matsumoto T, Kojima KK: Telomere-Specific Non-LTR Retrotransposons and Telomere Maintenance in the Silkworm, *Bombyx mori, Chromosome Res*., **13**, 455-467 (2005).

Katoh K, Kuma K, Toh H, Miyata T: MAFFT Version 5: Improvement in Accuracy of Multiple Sequence Alignment, *Nucleic Acids Res*., **33**, 511-518 (2005).

Katoh K, Kuma K, Miyata T, Toh H: Improvement in the Accuracy of Multiple Sequence Alignment Program MAFFT, *Genome Informatics*, **16**, 22-33 (2005).

Kojima KK, Fujiwara H: An Extraordinary Retrotransposon Family Encoding Dual Endonucleases, *Genome Res*., **15**, 1106-1117 (2005).

Kojima KK, Matsumoto T, Fujiwara H: Eukaryotic Translational Coupling in UAAUG Stop-Start Codons for the Bicistronic RNA Translation of Non-LTR Retrotransposon SART1, *Mol. Cell. Biol*., **25**, 7675-7686 (2005).

Kojima KK, Fujiwara H: Long-Term Inheritance of the 28S rDNA-Specific Retrotransposon R2, *Mol. Biol. Evol*., **22**, 2157-2165 (2005).

Nemoto W, Toh H: Prediction of Interfaces for Oligomerizations of G-protein Coupled Receptors, *Proteins*, **58**, 644-660 (2005).

Sato T, Yamanishi Y, Kanehisa M, Toh H: The Inference of Protein-protein Interactions by Co-evolutionary Analysis is Improved by Excluding the Information about the Phylogenetic Relationships, *Bioinformatics*, **21**, 3482-3489 (2005).

Thompson JD, Holbrook SR, Katoh K, Koehl P, Moras D, Eric Westhof, Poch O: MAO: a Multiple Alignment Ontology for Nucleic Acid and Protein Sequences, *Nucleic Acids Res*., **33**, 4164-4171 (2005).

[Others]

Nemoto W, Toh H: Interface Prediction for Class A GPCR Oligomers, *Tanpakushitsu Kakusan Koso*, **50**, 1382-1387 (2005) (in Japanese).

Nemoto W, Toh H: Bioinformatics, *Nippon Yakurigaku Zasshi*, **125**, 159-64 (2005) (in Japanese).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]
Center of Advanced Macromolecular Design, School of Chemical Engineering and Industrial Chemistry, The University of New South Wales

[Austria]
Institute for Physical Chemistry, University of Vienna

[Canada]
Chalk River Laboratories, National Research Council

Department of Chemistry and Faculty of Pharmacy, University of Montreal

Institute for Environmental Chemistry, National Research Council

[China, P. R.]
Department of Mathematics, Hong Kong Baptist University, Hong Kong

Department of Mathematics, The University of Hong Kong, Hong Kong

Department of Physical Chemistry, University of Science & Technology

Hefei National Laboratory for Physical Sciences at Microscale and Department of Chemistry, University of Science and Technology of China

Institute of Process Engineering, Chinese Academy of Sciences

School of Chemical Engineering and Technology, Tianjin University

State Key Laboratory of Applied Organic Chemistry, Lanzhou University

University of Science and Technology of China

[Estonia]
National Institute of Chemical Physics and Biophysics

[France]
Centre de Geostatistique, Ecole des Mines de Paris

Institut de Biologie Moleculaire et Cellulaire

Institut de Genetique et de Biologie Moleculaire et Celllulaire

Laboratoire CRISMAT-ENSICAEN, Université de Caen

[Germany]
Centre of Materials Science, Philipps University

Institut für Festkörperforschung, Forschungszentrum

Institute for Physical Chemistry, University of Göttingen

Institute of Physical Chemistry, Philipps University

Max Planck Institut fur Kernphysik

Max Planck Institute of Microstructure Physics

Physikalisches Institut, Albert-Ludwigs-Universität Freiburg

[Greece]
Department of Materials Science & Technology, Institute of Electronic Structure and Laser-FORTH, University of Crete

[Italy]
Dipartimento di Chimica Organica "A. Mangini", Alma Mater Studiorum - Universita di Bologna

Dipartimento di Ingegneria Chimica, Università degli Studi di Napoli "Federico II"

Istituto per i Materiali Compositi e Biomedici–CNR

Laboratory of Science, Materials and Nanotechnology, Nanoworld Institute, Dipartimento Architettura & Pianificaz, University of Sassari

[Korea, R.]
Department of Chemistry and Institute of Basic Science, Kyung Hee Univeristy

[New Zealand]
Department of Chemistry, University of Canterbury

[Philippines]
Industrial Technology Development Institute

[Poland]
Institute of Coal Chemistry, Polish Academy of Sciences, Gliwice

Medical Research Center, Polish Academy of Sciences, Warsaw

[Russia]
Department of Chemistry, Moscow State University

Joint Institute for Nuclear Research

[Spain]
Instituto de Química-Física “Rocasolano”, CSIC

[Switzerland]
Department of Chemistry and Applied Biosciences, Swiss Federal Institute of Technology (ETH)

Department of Organic Chemistry, University of Geneva

[Taiwan]
Department of Chemical Engineering, National Cheng Kung University

[Thailand]
Department of Chemistry, Faculty of Science, Mahasarakham University

Department of Chemistry, Faculty of Science, Mahidol University

[UK]
ISIS Facility, Rutherford Appleton Laboratory

School of Chemistry, University of Briston

[USA]
Chemical Sciences Division, Oak Ridge National Laboratory

Chemistry Department, Yale University

Department of Applied Physics, Stanford University

Department of Chemical Engineering, Clemson University

Department of Chemistry, North Carolina State University

Department of Chemistry, Northwestern University

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

Department of Chemistry, University of Tennessee

Department of Macromolecular Science and Engineering, Case Western Reserve University

Department of Physics and Astronomy, Johns Hopkins University

Lawrence Berkeley National Laboratory

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

NIST Center for Neutron Research, National Institute of Standards and Technology

Organosilicon Research Center, University of Wisconsin-Madison

Stanford Linear Accelerator Center, Stanford University

University of Calfornia Davis

*This list represents institutions where co-authors of the publications, listed up in P. 82-100, affiliate.

THESES

AHN, Young-Ock
D Agr, Kyoto University
"A New Class of Glycosidases Specific to Disaccharide Glycosides"
Supervisor: Prof SAKATA, Kanzo
24 January 2005

FADIL, Hicham
D Sc, Kyoto University
"Electron Cooling of Hot Ion Beams"
Supervisor: Prof NODA, Akira
23 March 2005

HAYASHIDA, Morihiro
D Inf, Kyoto University
"Computational Analysis and Inference of Protein-Protein Interactions from Domain Information"
Supervisor: Prof AKUTSU, Tatsuya
23 March 2005

IGARASHI, Yoshinobu
D Sc, Kyoto University
"The Evolutionary Repertoires of the Eukaryotic-Type ABC Transporters in Terms of the Phylogeny of ATP-binding Domains in Eukaryotes and Prokaryotes"
Supervisor: Prof KANEHISA, Minoru
23 November 2005

IKEGAMI, Masahiro
D Sc, Kyoto University
"Beam Dynamics in a Dispersionless Ion Storage Ring"
Supervisor: Prof NODA, Akira
23 March 2005

KAJIWARA, Takashi
D Sc, Kyoto University
"Studies on the Synthesis and Properties of Boron-stabilized Silyl Anions Utilizing Overcrowded Silylboranes"
Supervisor: Prof TOKITOH, Norihiro
23 March 2005

KAWAKAMI, Simpei
D Pharm Sc, Kyoto University
"Asymmetric Carbon-Carbon Bond Formation Based on Memory of Chirality"
Supervisor: Prof KAWABATA, Takeo
23 March 2005

KIWADA, Tatsuto
D Pharm Sc, Kyoto University
"Reversible Control of Helix Structure by External Stimuli and the Application as Functional Devices"
Supervisor: Prof SUGIURA, Yukio
23 March 2005

KOH, Kyoungmoo
D Eng, Kyoto University
"Precision Design of Organic/Inorganic Hybrid Materials by Living Radical Polymerization"
Supervisor: Prof FUKUDA, Takeshi
23 March 2005

KOJIMA, Masaaki
D Eng, Kyoto University
"Devulcanization and Recycling of Cross-Linked Natural Rubber Using Supercritical Carbon Dioxide"
Supervisor: Prof KOHJIYA, Shinzo
26 September 2005

KOSHINO, Masanori
D Sc, Kyoto University
"Electronic Structure Analysis of π–conjugated Organic Molecules by Electron Energy Loss Spectroscopy and Theoretical Interpretation of Local Atomic Site"
Supervisor: Prof ISODA, Seiji
23 March 2005

KOTERA, Masaaki
D Sc, Kyoto University
"Computational Assignment of the EC Numbers for Genomic-scale Analysis of Enzymatic Reaction"
Supervisor: Prof KANEHISA, Minoru
23 November 2005

KURATA, Atsushi
D Agr, Kyoto University
"Studies of Novel Enzyme Catalyzing Asymmetric Reduction of 2-Chloroacrylic Acid"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2005

KUSUMOTO, Tomokazu
D Pharm Sc, Kyoto University
"Coloration of Molecular Information by Functional Phenolphthaleins"
Supervisor: Prof KAWABATA, Takeo
23 March 2005

KWAK, Mi-Sun
D Agr, Kyoto University
"Studies of Protein Systems Depending on Cysteine Desulfurase and Selenocysteine Lyase"
Supervisor: Prof ESAKI, Nobuyoshi
25 July 2005

LEE, Yangsoo
D Eng, Kyoto University
"Studies on Synthesis, Properties, and Reactions of Alkylated Fullerene Cations"
Supervisor: Prof KOMATSU, Koichi
23 March 2005

MASAI, Hirokazu
D Eng, Kyoto University
"Studies on the Organically-Modified Polysiloxane Low-Melting Glasses"
Supervisor: Prof YOKO, Toshinobu
21 May 2005

MORI, Ryohei
D Eng, Kyoto University
"Preparation and Photoelectrochemical/Photocatalytic Properties of Sol-Gel Derived TiO_2 Thin Film with Spinodal Phase Separation Structure"
Supervisor: Prof YOKO, Toshinobu
21 May 2005

MURAMATSU, Hisashi
D Agr, Kyoto University
"Studies of Enzymes Useful for Production of Optically Active *N*-Alkyl Amino Acids and Cyclic Imino Acids"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2005

NAGAI, Yasuharu
D Sc, Kyoto University
"Mechanisms and Kinetics of Noncatalytic Ether Reaction in Supercritical Water"
Supervisor: Prof NAKAHARA, Masaru
23 May 2005

NAITO, Kanako
D Sc, Kyoto University
"Iron Uptake by Eukaryotic Phytoplankton under Iron-Deficient Conditions"
Supervisor: Prof SOHRIN, Yoshiki
23 March 2005

NAKASE, Ikuhiko
D Pharm Sc, Kyoto University
"Internalization Mechanisms of Basic Peptide Vectors and Intracellular Delivery of Bioactive Molecules"
Supervisor: Prof SUGIURA, Yukio
23 March 2005

NOMURA, Wataru
D Pharm Sc, Kyoto University
"Investigation of Effects of the Linker Region of Zinc Finger Proteins on DNA Binding"
Supervisor: Prof SUGIURA, Yukio
23 March 2005

OGAWA, Kohei
D Eng, Kyoto University
"Synthesis and Properties of Novel Hydrocarbons Containing Rigid Cage Frameworks"
Supervisor: Prof KOMATSU, Koichi
23 March 2005

POOMPRADUB, Sirilux
D Eng, Kyoto University
"Structure and Physical Properties of Natural Rubber Based Composite Materials"
Supervisor: Prof KOHJIYA, Shinzo
26 September 2005

SAITO, Shigeki
D Agr, Kyoto University
"Studies on (+)-Abscisic Acid 8'-Hydroxylase, a Key Enzyme in the Catabolism of Abscisic Acid"
Supervisor: Prof SAKATA, Kanzo
23 May 2005

SHIMOTOYODOME, Akira
D Agr, Kyoto University
"Physiological Studies of Colonic Mucus Secretion in Rats"
Supervisor: Prof ESAKI, Nobuyoshi
24 November 2005

SHINOHARA, Akihiro
D Sc, Kyoto University
"Systematic Studies on the Kinetically Stabilized Silaaromatic Compounds"
Supervisor: Prof TOKITOH, Norihiro
23 March 2005

TAJIMA, Tomoyuki
D Sc, Kyoto University
"Studies on the Synthesis and Properties of Metallacyclopropabenzenes Using Dilithiometallanes"
Supervisor: Prof TOKITOH, Norihiro
23 March 2005

TAKAJO, Daisuke
D Sc, Kyoto University
"Studies on Initial Stage of Multi-layer Growth of Organic Molecules by Scanning Tunneling Microscopy"
Supervisor: Prof ISODA, Seiji
23 March 2005

TANAKA, Hiroyuki
D Pharm Sc, Kyoto University
"Studies on Synthesis and Function of 1,4-Connected Oligonaphthalenes"
Supervisor: Prof KAWABATA, Takeo
23 March 2005

YAMANISHI, Yoshihiro
D Sc, Kyoto University
"Development of Methods for Analyzing the Correlation between Heterogeneous Genomic Data and Their Application to Inferring Protein Network"
Supervisor: Prof KANEHISA, Minoru
23 November 2005

YOSHIMUNE, Kazuaki
D Agr, Kyoto University
"Studies on Biochemistry and Application of Hsp70 Family Proteins"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2005

YOSHIOKA, Taiyo
D Eng, Kyoto University
"Morphological Studies on High-Speed-Spun Fibers of Aromatic Polyesters"
Supervisor: Prof KOHJIYA, Shinzo
23 March 2005

YOW, Geok-Yong
D Agr, Kyoto University
"Enzymological Studies of D-Amino Acid *N*-Acetyltransferase from *Saccharomyces cerevisiae*"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2005

THE 105TH ICR ANNUAL SYMPOSIUM

SEMINARS

MEETINGS AND SYMPOSIUMS

THE 105TH ICR ANNUAL SYMPOSIUM

(2 December 2005)

ORAL PRESENTATION

ONO, Teruo (Magnetic Materials)
"Manipulation of Magnetization by Spin-current"

NISHIDA, Koji (Polymer Materials Science)
"Inversion of Interaction and Structure Formation in Polyelectrolyte Solution"

TSUGE, Tomohiko (Molecular Biology)
"A Master Regulator Linking Plant Environmental Responses to Morphogenesis Signaling"

HATTORI, Masahiro (Bioknowledge Systems)
"Analysis of Atom Transformation Patterns in Enzymatic Reactions Based on the Comparison of Chemical Compound Structures"

NORISUYE, Kazuhiro (Hydrospheric Environment Analytical Chemistry)
"Chemical Method for Analysis of Sources of Plutonium Isotopes in the Ocean"

- The ICR Award for Young Scientist -
TAKEDA, Nobuhiro (Organoelement Chemistry)
"Synthesis of Novel Organosilicon Species by Taking Advantage of a Silylene Bearing Bulky Substituents and the Elucidation of Their Properties"

- The ICR Award for Students -
MURATA, Michihisa (Structural Organic Chemistry)
"Organic Synthesis of Fullerene C_{60} Encapsulating Molecular Hydrogen"

KAN, Daisuke (Advanced Solid State Chemistry)
"Blue-Light Emission at Room Temperature from Ar^{+}- Irradiated $SrTiO_3$"

- The ICR Grants for Young Scientists -
TOKUDA, Yomei (Inorganic Photonics Materials)
"Studies of Glass Formation Process for Organic & Inorganic Hybrid Low-melting Glass and Application for Light Functionality Devices"

SHIMIZU, Seiji (Laser Matter Interaction Science)
"Development and Application for Advanced Laser Mass Spectrometry"

MIHARA, Hisaaki (Molecular Microbial Science)
"Analysis of Metabolic Pathways by Collaboration between Bioinformatics and Biochemistry"

OHNO, Kohji (Chemistry of Polymer Materials)
"Newly Development of Magnetically Tunable Colloidal Crystals"

POSTER PRESENTATIONS

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

— Organoelement Chemistry —

LW "Synthesis of Nobel Organic Compounds Containing Heavier Elements by Taking Advantage of Kinetic Stabilization and the Elucidation of Their Properties"

GE NAGAHORA, Noriyoshi; SASAMORI, Takahiro; TOKITOH, Norihiro
"Syntheses, Structures, and Properties of Kinetically Stabilized 1,1'-Bis(diphosphenyl)ferrocenes"

GE TAJIMA, Tomoyuki; TAKEDA, Nobuhiro; SASAMORI, Takahiro; TOKITOH, Norihiro
"A Kinetically Stabilized Tin-Tellurium Double-bond Compound: Synthesis, Structure, and Reactivities"

— Structural Organic Chemistry —

LT YAMAZAKI, Daisuke; TANINO, Nobuhide; NISHINAGA, Tohru; KOMATSU, Koichi
"π-Dimer Formation of Radical-Cation Salt of Terthiophene End-Capped with Bicyclic Frameworks"

GE MAEDA, Shuhei; MURATA, Michihisa; MURATA, Yasujiro; KOMATSU, Koichi
"Encapsulation of Two Hydrogen Molecules into an Open-Cage C_{70} Derivative"

GE TERAYAMA, Miki; MIYATA, Yasuo; KOMATSU, Koichi
"Synthesis and Properties of Ferrocene Connected with Diphenylterthiophene by Alkyl Chain"

GE MATSUBARA, Hiroaki; KITAGAWA, Toshikazu; KOMATSU, Koichi
"Synthesis of Novel Ferrocene-Terminated Thiols and the Electrochemical Properties of Their Monolayers on Au(111)"

— Synthetic Organic Chemistry —

LT MURAMATSU, Wataru; NISHIO, Tadashi; KAWABATA, Takeo
"Regioselective Acylation of Sugars by Chiral Nucleophilic Catalysts"

GE MONGUCHI, Daiki; KAWABATA, Takeo
"Asymmetric Intramolecular Conjugate Addition of Chiral Enolates via Racemization-Free Equilibrium"

— Advanced Inorganic Synthesis —

LW "Activity Report: Advanced Inorganic Synthesis Laboratory"

LT AZUMA, Masaki
"Magnetic Ferroelectrics Bi,Pb-3d Transition Metal Perovskites"

— Chemistry of Polymer Materials —

LT YOSHIKAWA, Chiaki; GOTO, Atsushi; TSUJII, Yoshinobu; FUKUDA, Takeshi
"Novel Biointerface with Concentrated Polymer Brush - Protein Repellency of Concentrated Brush by Size-Exclusion Effect"

GE ZUSHI, Hirokazu; GOTO, Atsushi; FUKUDA, Takeshi
"Novel Living Radical Polymerization Catalyzed by Germanium and Tin Compounds"

GE OKAYASU, Kenji; TSUJII, Yoshinobu; FUKUDA, Takeshi
"Ultra-Low Frictional Properties of High-Density Polymer Brushes in a Good Solvent"

— Chemistry of Polymeric Functionality Materials —

GE TOGAI, Manabu; SENOO, Kazunobu; KOHJIYA, Shinzo
"Increase of Lithium-ion Conductivity by Uniaxial Stretching of PEO/Ionic Salt Solid Solution"

— Inorganic Photonics Materials —

LT MAEDA, Takahiro; TAKAHASHI, Masahide; YAO, Jianxi; TOKUDA, Yomei; NISHII, Junji; YOKO, Toshinobu
"Fabrication of TiO_2 Periodic Structure by the Photopolymerization-induced Phase Separation Method"

GE MIZUNO, Megumi; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu
"Organically-modified Silicophosphate Prepared via Non-aqueous Acid-base Reaction"

GE KUNIYOSHI, Minoru; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu
"Preparation of Organic-inorganic Hybrid Polysiloxane Glasses by Sol Concentration Method"

— Biofunctional Design-Chemistry —

LT TADOKORO, Akiko; NAKASE, Ikuhiko; KAWABATA, Noriko; TAKEUCHI, Toshihide; FUTAKI, Shiroh
"Cellular Uptake of Arginine-rich Peptides: Proteoglycans and R8"

GE HIGASHI, Chika
"Protein-protein Interaction between DNA Binding Zinc Finger Domains"

— Chemistry of Molecular Biocatalysts —

LT SAINO, Hiromichi; FUJIHARA, Fuyuki; MIZUTANI, Masaharu; HIRATAKE, Jun; SAKATA, Kanzo
"Elucidation of Substrate Recognition Mechanism by Disaccharide-specific Diglycosidases from Plants"

GE HASEGAWA, Atsuko; NAKAGAWA, Yuichi; HIRATAKE, Jun; SAKATA, Kanzo
"Directed Evolution of Lipase for Improved Amide-hydrolyzing Activity -Suturation Mutagenesis at Substrate Binding Site-"

GE HAN, Liyou; KAMIYAMA, Akane; HIRATAKE, Jun; SAKATA, Kanzo
"Probing the Catalytic Mechanism of Gamma-glutamyl Transpeptidase by Gamma-phosphono Glutamate Analogs as Mechanism-based Inhibitors"

— Molecular Biology —

LT KUSANO, Hiroaki; YASUDA, Keiko; AKI, Shiori; OKA, Atsuhiro; AOYAMA, Takashi
"Identification of the Arabidopsis Phosphatidyl Inositol 4-phosphate 5-kinase Gene Regulating Root-hair Development"

— Chemical Biology —

LT SATO, Ayato; KAWAZOE, Yoshinori; UESUGI, Motonari
"Design and Synthesis of Small Molecule Transcription Factors"

— Molecular Materials Chemistry —

LW "Structure and Dynamics of Functional Molecular Materials"

— Hydrospheric Environment Analytical Chemistry —

LT MOCHAMAD, Lutfi Firdaus; NORISUYE, Kazuhiro; SOHRIN, Yoshiki
"Development of a Solid-phase Extraction Method for the Determination of Zr, Hf, Nb, Ta and W in Seawater Using Inductively Coupled Plasma–Mass Spectrometry"

LT NAKATSUKA, Seiji
"Geochemistry of Trace Metals during an In-situ Iron Enrichment in Subarctic North Western Pacific"

— Solution and Interface Chemistry —

LT YOSHIDA, Ken; WAKAI, Chihiro; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru
"Translational and Rotational Dynamics of Sub- and Supercritical Water Using High-Temperature High-Pressure Multinuclear NMR Probe"

GE MOROOKA, Saiko; WAKAI, Chihiro; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru
"A New Hydrothermal C1 Chemistry: C-C bond Formation and Disproportionations from Formaldehyde and Formic Acid"

— Molecular Microbial Science —

LT KUROKAWA, Suguru
"Selenium Recognition Mechanism"

GE JITSUMORI, Keiji; OMI, Rie; KURIHARA, Tatsuo; MIYAHARA, Ikuko; HIROTSU, Ken; ESAKI, Nobuyoshi
"Cleavage Mechanism of Carbon-fluorine Bond by Fluoroacetate Dehalogenase"

— Polymer Materials Science —

LW "Detailed Analysis for Super-structure of Polymers"

GE TAKAYAMA, Yoshiyuki; OGINO, Yoshiko; MATSUBA, Go; NISHIDA, Koji; KANAYA, Toshiji
"Formation of Meso-phase and Crystallization of Isotactic Polystyrene under Shear"

GE TSUBOUCHI, Tsuyoshi; NISHIDA, Koji; KANAYA, Toshiji
"Phase Separation and Aggregation of Hetero Polyelectrolyte Solutions"

GE SAKAMOTO, Shinya; OGINO, Yoshiko; MATSUBA, Go; NISHIDA, Koji; KANAYA, Toshiji
"Effect of Ultra High Molecular Weight Component in Crystallization of Polyethylene under Shear Flow"

— Molecular Rheology —

GE TAKASHIMA, Ryota; MATSUMIYA, Yumi; INOUE, Tadashi; WATANABE, Hiroshi; KIHARA, Shinichi; OSHIMA, Masahiro
"Dielectric Behavior of Polyisoprene under Pressurized Carbon Dioxide"

GE MATSUMOTO, Manabu; MATSUMIYA, Yumi; INOUE, Tadashi; WATANABE, Hiroshi
"Nonlinear Rheology and Structure of Multi Block Copolymer"

GE TAGASHIRA, Masao; MATSUMIYA, Yumi; INOUE, Tadashi; WATANABE, Hiroshi
"Rheology and Rheo-dielectric Behavior of Lithium Perchlorate/Polyethyrene Oxide System"

GE OISHI, Yohei; WATANABE, Hiroshi
"Dynamics of Living Polybutadiene Anion"

— Molecular Aggregation Analysis —

LT TSUTSUMI, Junya; KATO, Shigeki; SATO, Naoki
"Ab Initio Calculation of Lattice Energy of Organic Molecular Crystals – Electronic Polarization Effect –"

GE ASAMI, Koji
"Dielectric Dispersion of Lysed Erythrocytes"

— Supramolecular Biology —

LT TAKAHARA, Keigo; TAKEUCHI, Ken-ichi; UMEDA, Masato
"Study for Function of Fatty Acid Desaturase in Organisms"

LT INADOME, Hironori; KATO, Utako; UMEDA, Masato
"Membrane Lipid Dynamics; Its Role in Regulation of Cell Morphology"

— Particle Beam Science —

LW "Research Activity at Particle Beam Science Laboratory"

LT IKEGAMI, Masahiro
"Beam Cooling Simulation at Ion Storage Ring S-LSR"

LT FADIL, Hicham
"Electron Cooling Experiments at S-LSR"

GE SHIRAI, Toshiyuki
"Beam Commissioning of the Ion Cooler Ring, S-LSR"

— Laser Matter Interaction Science —

LW "Activities of Laser-Matter Interaction Science"

GE HASHIDA, Masaki; SHIMIZU, Seiji; SAKABE, Shuji
"Femtosecond Laser Ablation of Material Surface"

— Electron Microscopy and Crystal Chemistry —

LT JIU, Jinting
"Dye-sensitized Solar Cell Based on TiO_2 Film Composed of Nanaorods"

LT NEMOTO, Takashi
"Regularly-shaped Diacetylene Nano-structures on Surfaces"

— Structural Molecular Biology —

LT HATA, Yasuo; FUJII, Tomomi
"Structural Analysis of Molecular Mechanism of CPY Inhibition by Protein I^C"

— Organic Main Group Chemistry —

LW "Organic Main Group Chemistry Lab in 2005"

GE FUKAZAWA, Aiko; HIRORI, Hideki; INOUYE, Hideyuki; TSUJI, Hayato; KANEMITSU, Yoshihiko; TAMAO, Kohei
"Photophysical Properties of Oligosilanes Based on the Bicyclic Trisilane Units"

GE INOUE, Tomoyuki
"Synthesis, Structure and Properties of Transition Metal-Phosphasilatriptyene Complexes"

GE KOMATSU, Shigeo; TSUJI, Hayato; SAEKI, Tomoyuki; KANDA, Yasuhisa; UMEHARA, Teruhiko; TAMAO, Kohei
"Development of Double *Ortho*-Lihtiation of Diphenylphosphoryl Amide and Benzophenone"

— Advanced Solid State Chemistry —

LW "Transition Metal Oxides - Functions and Synthesis -"

GE YAMAMOTO, Shinpei
"Synthesis of $L1_0$-FePt Nanoparticle by SiO_2 Nanoreactor Method"

— Organotransition Metal Chemistry —

LW "Recent Topics in Organotransition Metal Chemistry Laboratory"

GE MUTOH, Yuichiro; YAMAMOTO, Yasutaka; NAGAO, Masato; KATAYAMA, Hiroyuki; OZAWA, Fumiyuki
"Oligo(phenylene vinylene)s: Stereocontrolled Synthesis and Photochemical Properties"

GE YOSHIMURA, Ken-ichi; UEHIRA, Kosei; TAKANO, Masato; OKAZAKI, Masaaki; OZAWA, Fumiyuki
"Systematic Synthesis and Property of Haloacetylene-Coordinated Tetrairon Clusters"

— Photonic Elements Science —

LW "Recent Research Results in Photonic Elements Science"

— Bioknowledge Systems —

LW "Integrated Database for Genome and Chemical Information: KEGG and Prediction of Drug Degradation Pathways"

— Biological Information Networks —

LT K. C., Dukka Bahadur; AKUTSU, Tatsuya
"Clique Based Algorithms for Protein Threading with Constraints"

— Pathway Engineering —

LT ZHU, Shanfeng; MAMITSUKA, Hiroshi
"Mining Biomedical Co-occurrence Data Using a Probabilistic Model"

— Bioinformatics Training Unit —

LT ICHIHARA, Hisako; KUMA, Kei-ichi; TOH, Hiroyuki
"Evolutionary Analysis of Proteins Relevant to Quorum Sensing"

SEMINARS

Dr AGUILAR NETZ, Daili Jacqueline
Microbiology, Philipps-University Marburg, Germany
"Iron-Sulfur Biogenesis in Yeast Cytosol"
22 March 2005

Prof AHARONY, Amnon
Tel Aviv University, Ben Gurion University, Israel
"What is Really Measured in the Mesoscopic Aharonov-Bohm Interferometer?"
24 October 2005

Dr ALDABBAGH, Fawaz
National University of Ireland, Ireland
"The Controlled Synthesis of Stimuli-Sensitive Materials"
5 December 2005

Prof ATTFIELD, John P
University of Edinburg, UK
"The Chemical Control of Electron Oxides"
25 January 2005

Prof BABONNEAU, Florence
Prof BONHOMME, Christian
Chimie de la Matière Condensée, Université Paris 6, France,
"Advanced Solid State NMR for the Characterisation of Sol-gel Derived Materials"
7 November 2005

Prof BALTA-CALLEJA, J. Francisco
Instituto de Estructura de la Materia, CSIC, Spain
"Micromechanical Properties of Polymers Relating to Nanostructure"
31 May 2005

Prof BRAUNSTEIN, Pierre
Universite Louis Pasteur, Strasubourg, Cédex, France
"From Bimetallic Complexes, Chains and Clusters to Nanomaterials"
20 September 2005

Prof BUBACK, Michael
Institute for Physical Chemistry, University of Göttingen, Germany
"Recent Studies on the Kinetics of Free Radical Polymerization"
19 August 2005

Prof BUCKEL, Wolfgang
Microbiology, Philipps-University Marburg, Germany
"Reverse Electron Transfer in Anaerobic Bacteria"
19 March 2005

Dr CHAU, Pak-Lee
Pasteur Institute, France
"Molecular Recognition - Beyond the Receptor"
12 January 2005

Prof CHOU, Li-Jen
National Tsing-Hua University, Taiwan
"Synthesis and Characterization of $TaSi_2$, $HfSi_2$, GaN, WO_3 and Fe_2O_3"
12 September 2005

Dr COUPRIE, Marie-Emmanuelle
LURE, France
"ARC-EN-CIEL"
24 October 2005

Dr DEMÉ, Bruno
Institut Laue-Langevin, Grenoble, France
"Small-angle Neutron Scattering of Model Biological Membranes Confined in Nanoporous Alumina"
13 June 2005

Prof DRIESS, Matthias
Technical University Berlin, Germany
"From Metal-Oxo-Clusters to Challenges in Catalysis"
30 November 2005

Prof ENTIN-WOHLMAN, Ora
Tel Aviv University, Israel
"ac spin-Hall Effect of Localized Electrons"
24 October 2005

Prof ERKER, Gerhard
Organisch-Chemisches Institut, Universitat Munster, Munster, Germany
"Syntheses and Reactions of Bifunctional Metallocene Complexes"
7 June 2005

Prof GAUZZI, Andrea
Institut de Minéralogie et de Physique des Milieux Condensés Université de Paris 6 "Pierre et Marie Curie", Paris, France
"Unusual e_g $3d$ x^2-y^2 Orbital Ordering and Low-energy Excitationsin the CE Structure of $NaMn_7O_{12}$"
2 November 2005

Prof GLEITER, Rolf
Organisch-Chemisches Institut, University of Heidelberg, Heidelberg, Germany
"From Superphanes to Beltenes"
27 October 2005

Prof GOLDING, Bernard
Organic Chemistry, University of Newcastle upon Tyne, England
"The Remarkable Metabolism of Chloroprene: A Big Story from a Little Molecule"
19 March 2005

Dr GUTIERREZ, Aldo F.
Department of Biochemistry, University of Leicester, England
"From Binding Energy to Protein Dynamics in Redox Enzymes"
19 April 2005

Prof HAN, Kyou Hoon
Korea Research Institute of Bioscience and Biotechnology, Korea
"An NMR Approach to Study Unstructured Proteins; a Case Study on p53-mdm2"
8 November 2005

Prof HANGST, Jeffrey
University of Aarhus, Denmark
"Project ALPHA - A New Experiment for Antihydrogen Production and Trapping"
17 March 2005

Prof HILLEBRANDS, Burkard
Technische Universitaet Kaiserslautern, Germany
"Optical Detection of Spin Dynamics in Magnetic Nanostructures "
11 April 2005

Prof HOFMANN, Ingo
GSI, Germany
"Recent Developments in Beam Physics at GSI"
2 March 2005

Prof HUDECZ, Ferenc
Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary
"Synthesis and Characterization of Cyclic Epitope Peptide Dimers, Conjugates from Glycoprotein D of Herpes Simplex Virus Type 1"
26 October 2005

Prof INNOCENZI, Plinio
University of Sassari, Italy
"Organic-inorganic Hybrid Materials Prepared by Sol-gel Process"
7 Feburuary 2005

Dr KATO, Atsushi
Research Department, Nissan Arc, Ltd., Yokosuka, Japan
"Analysis of Ruptured Surface and Cross Section of Polymeric Materials"
17 June 2005

Prof KAWANABE, Keiichi
Graduate School of Medicine, Kyoto University, Kyoto, Japan
"Durability of Artificial Joint"
26 November 2005

Prof KISHIDA, Akio
Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, Japan
"Biocompatibility and Concentrated Polymer Brush"
26 November 2005

Prof KLEIN, Michael L.
University of Pennsylvania, USA
"Computer Simulation of Self-Assembling Amphiphilic Systems: From Natural to Synthetic Membranes"
14 April 2005

Prof KRÄTSCHMER, Wolfgang
Max-Plank Institute für Kernphysik, Heidelberg, Germany
"IR and UV-VIS Spectroscopy on Odd Carbon Chain Molecules"
24 January 2005

Senior Researcher LAPARRA, Hélène
Research Department of Meristem Therapeutics, Clermont-Ferrand, France
"Large Scale Production of Recombinant Therapeutic Proteins in Plants"
8 April 2005

Dr LIZ-MARZÁN, Luis M
Department of Physical Chemistry, University of Vigo, Vigo, Spain
"Tailoring Surface Plasmons through the Morphology and Assembly of Metal Nanoparticles"
26 July 2005

Dr MAGONOV, Sergei
Digital Instruments / Veeco Metrology Group, Santa Barbara, CA, USA
"Modern Trends in Atomic Force Microscopy of Polymers"
15 July 2005

Prof MARCHESSAULT, Robert H
Xerox Research Center of Canada, Montreal, Canada
"Fishing for Proteins with Magnetized Cellulose"
26 October 2005

Dr MARGETIC, Davor
Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Zagreb, Croatia
"Cycloaddition Molecular "Glues" and Their Synthetic Applications"
3 February 2005

Prof MAROM, Gad
The Hebrew University of Jerusalem, Israel
"Flow Induced Crystallization of Polymers"
28 April 2005

Prof MATYJASZEWSKI, Krzysztof
Department of Chemistry, Carnegie Mellon University, USA
"Well-Defined Hybrid Polymers – Materials for the Future"
17 November 2005

Prof MEZO, Gabor
Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary
"Drug Targeting by Peptide Conjugates"
26 October 2005

Prof MINAGAWA, Masao
Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan
"Paleoenvironmental Changes Reconstructed Using Chemical Proxies in Sediment Cores"
2 September 2005

Vis Prof NISHIO, Taichi
Sanzen Kako Co. Ltd.
"Present Situation and Vision for Polyolefin as a Background of Social Environment"
11 November 2005

Prof OTOMO, Toshiya
High Energy Accelerator Research Organization, Ibaraki, Japan
"J-Parc: Construction of the World-Best Proton Accelerator"
7 February 2005

Dr PARKIN, Stuart
IBM Almaden Research Center, USA
"Magnetic Shift Register - a Novel Storage Class Memory"
14 June 2005

Prof PARMAR, Virinder S.
University of Dehli, India
"Novel Natural Products and their Biological Activity"
25 March 2005

Dr PIERIK, Antonio J.
Microbiology, Philipps-University Marburg, Germany
"Nicotinate Metabolism"
22 March 2005

Prof POEPPELMEIER, Kenneth R.
Department of Chemistry, Northwestern University, Evanston, Illinois, USA,
"Metal Oxide Surfaces: God Made the Solid State. He Left the Surface to the Devil...Wolfgang Pauli"
16 March 2005

Prof RUBIN, Yves
Department of Chemistry and Biochemistry and Exotic Materials Institute, University of California, Los Angeles, USA
"The Inside and Out of Fullerene Chemistry"
28 July 2005

Prof RUSSELL, Gregory T.
Department of Chemistry, University of Canterbury, New Zealand
"Do We Really Understand the Kinetics of Emulsion Polymerization?"
12 April 2005

Prof SALJE, Ekhard K.H.
Department of Earth Science, Cambridge University, Cambridge, UK
"Self Organized Structures in Ferroelastic and Co-elastic Systems"
15 September 2005

Dr SAMOSON, Ago
National Institute of Chemical Physics and Biophysics, Estonia
"Advances in Sample Spinning Solid State NMR and Related Applications"
14 November 2005

Dr SATO, Takaya
Department of Materials Engineering, Tsuruoka National College of Technology, Yamagata, Japan
"Ion Channel by Polymerizable Ionic Liquid"
26 November 2005

Prof SCHICK, Cristoph
University of Rostock, Germany
"Reorganization of Polymer Crystals Studied by Fast Scanning Calorimetry (10,000K/s)"
18 February 2005

Dr SELEZNEV, Igor
Joint Institute for Nuclear Research, Russia
"Coupling Motion in the LEPTA Ring with Focusing by Longitudinal Magnetic Field"
28 November 2005

Dr SELMER, Thorsten
Microbiology, Philipps-University Marburg, Germany
"Clostridial Arylacetate Decarboxylases: Evidence for Complex Regulation of a Putative Self-defense System in Anaerobes"
19 March 2005

Assoc Prof SERINO, Giovanna
University of Rome, La Sapienza, Rome, Italy
"Uncovering Novel COP9 Signalosome-dependent Pathways in *Arabidopsis*"
22 August 2005

Prof SHEVELKO, V.P.
Lebedev Physical Institute, Russia
"Target-density Effects in Collisions of Fast Ions with Solid Targets"
26 October 2005

Prof SUZUKI, Hisanori,
University of Verona, Italy
"STAT1 as A New Target of Anti-Inflammatory Treatment"
"Alfa-Bisabolol: A New Anti-Cancer Drug? "
30 November 2005

Prof SOKOLOV, P. Alexi
Department of Polymer Science, The University of Akron, USA
"When does a Molecule Become a Polymer?"
9 September 2005

Vice-Director TABATA, Satoshi
Kazusa DNA Research Institute, Kisarazu, Japan
"Genome Analysis of *Lotus japonicus* and Common DNA Markers for Genome Comparison among Leguminous Plants"
4 March 2005

Prof TANG, Pei
University of Pittsburgh School of Medicine, USA
"Protein Dynamics and Molecular Mechanisms of General Anesthesia"
28 February 2005

Prof THEOPOLD, Klaus H.
Department of Chemistry & Biochemistry, Center for Catalytic Science and Technology, University of Delaware, Newark, Delaware, U.S.A.
"Dioxygen Activation with tris(pyrazolyl)-borate Metal Complexes"
15 January 2005

Assist Prof TOMODA, Kiichiro
Nara Institute of Science and Technology, Ikoma
"Roles of Jab1 ($p27^{Kip1}$ binding protein) in Mammals: Cell Transformation and Stem Cell Maintenance"
14 December 2005

Prof TYKWINSKI, Rik R
Department of Chemistry, University of Alberta, Edmonton, Canada
"Modeling Carbyne: Surprising Properties of Conjugated Polyynes"
29 January 2005

Dr VANA, Philipp
Institute for Physical Chemistry, University of Göttingen, Germany
"Kinetics and Applications of Controlled Radical RAFT Polymerization"
26 November 2005

Prof WANG, Hao
Beijing University of Technology, China
"Microwave-assisted Chemical Bath Deposition of Luminescent Eu:YVO_4 Thin Films"
26 July 2005

Dr YAMAMOTO, Kazuya
Graduate School of Science and Engineering, Kagoshima University, Kagoshima, Japan
"Biointerface"
26 November 2005

Prof YOSHIOKA, Keiko
Department of Botany, University of Toronto, Toronto, Canada
"cpr22-mediated Pathogen Resistance Signaling in *Arabidopsis*"
19 May 2005

Prof ZIPSE, Hendrik
Ludwig-Maximilians-Universität in München, Germany
"Catalysis in Acyl Transfer Reactions"
16 September 2005

MEETINGS AND SYMPOSIUMS

The 4th International Symposium of the Kyoto COE Project "Elements Science": "Elements Selection Rule and Materials Science" and The 2nd Internaional Symposium of International Research Center for Elements Science
Organized by TAMAO, Kohei and TOKITOH, Norihiro
6-7 January 2005 (Kyoto, Japan)

Develeopment of 3d Transition-metal Oxides with Oxygen Holes
Organized by TAKANO, Mikio
29 January 2005 (Kyoto, Japan)

Assoc Prof AZUMA, Masaki
Kyoto University
"Bi,Pb 3d Transition Metal Perovskites"

Prof WADATI, Hiroki
Tokyo University
"Electronic Structure of $Bi_{1-x}La_xNiO_3$"

Dr MASUNO, Atsunobu
Kyoto University
"Control of Physical Properties of Micro-fabricated Perovskite-type Manganese Oxide Thin Films by Spin-polarized Current"

Prof FUJIMORI, Atsushi
Tokyo University
"Raman Spectroscopy of Fe Perovskite"

Prof OKAMOTO, Yoshihiko
Tokyo University
"Physical Properties of Ir Oxide with Hyper-kagome Lattice, $Na_4Ir_3O_8$"

Dr SAITO, Takashi
Kyoto University
"Introduction and the Substitution Effect of $SrCo_6O_{11}$"

Prof MUKUDA, Hidekazu
Osaka University
"Co-NMR Study of $SrCo_6O_{11}$"

Dr ISHII, Fumiyuki
National Institute of Advanced Industrial Science and Technology
"First Principle Calculation of $SrCo_6O_{11}$:Magnetic and Electronic Structures"

Assoc Prof TERASHIMA, Takahito
Kyoto University
"Light Emission from $SrTiO_3$"

Prof NOHARA, Minoru
Tokyo University
"Metal-insulator Transition and Thermoelectric Properties of $Sr_{1-x}Rh_2O_4$"

Prof TAKEDA, Yasuo
Mie University
"Anomalous Thermal Expansion and Jahn-Teller Effect of $GdMnO_3$ Compounds"

Dr YAMAMOTO, Shinpei
Kyoto University
"Synthesis of Solvent-Dispersed $L1_0$-FePt Nanocrystals"

Prof KATAYAMA, Naoyuki
Tokyo University
"Superconductivity in Hydrated Layered Transition Metal Sulfides"

Prof ARAI, Yuhki
Tokyo University
"Magnetic Properties of Hydrated Layered Ni Oxide"

21st Century COE on Kyoto University Alliance for Chemistry "Fine Organic Synthesis Seminar"
Organized by KAWABATA, Takeo; TSUBAKI, Kazunori; TOKITOH, Norihiro: OZAWA, Fumiyuki: KOMATSU, Koichi
4-5 February 2005 (Kyoto, Japan)

Oral Presentations
Prof ISHIHARA, Kazuaki
Nagoya University
"Catalysts for Dehydration toward the Development of Green Chemical Processes"

Assoc Prof TOMOOKA, Katsuhiko
Tokyo Institute of Technology
"Chemistry of Chiral Small Molecules with No Central Chirality at Carbons"

Dr TAKASU, Kiyosei
Tohoku University
"Rapid and Efficient Synthesis of Multisubstituted Cyclic Compounds: Domino-Reactions, Multi-Component Coupling Reactions, and Organoacid Catalysis"

Prof IWASAWA, Shinji
Tokyo Institute of Technology
"Creation and Reactions of Tungsten-Containing 1,3-Dipoles"

Dr KAN, Toshiyuki
Tokyo University
"Synthesis of Isoquinoline Alkaloids"

Assoc Prof TANINO, Keiji
Hokkaido University
"Development of Advanced Addition Reactions and their Application to Natural Product Synthesis"

Prof SASAI, Hiroaki
Osaka University
"Development of Asymmetric Catalysts with Dual Functional Activation"

Assoc Prof TSUBAKI, Kazunori
Kyoto University
"Fine Organic Synthesis of Chiral Oligonaphthalenes"

Assoc Prof NAKAMURA, Masaharu
Tokyo University
"Development of Catalytic Addition Reactions of Carbonyl Compounds to Simple Alkenes and Alkynes"

Assoc Prof SHINOKUBO, Hiroshi
Kyoto University
"Development of New Reactions Promoted in Aqueous Media"

Assoc Prof OI, Shuichi
Tohoku University
"Regioselective Substitution of Aromatic C-H Bonds by Aryl Groups Promoted by Transition Metal Catalysts"

Prof NISHIDA, Atsushi
Chiba University
"Asymmetric Total Synthesis of Alkaloids with Complex Ring System"

21st Century COE on Kyoto University Alliance for Chemistry "The 2nd Organoelement Chemistry Seminar"
Organized by OZAWA, Fumiyuki; KATAYAMA, Hiroyuki; TOKITOH, Norihiro; TAKEDA, Nobuhiro
5 March 2005 (Kyoto, Japan)

Chemistry and Physics of 3d Transition Metal Oxides Equipped with Deep 3d Levels: Search for New Materials and New Functions
Organized by TAKANO, Mikio
20 May 2005 (Kyoto, Japan)

Prof SHIMAKAWA, Yuichi
Kyoto University
"Functional Oxides for Future Memory Devices"

Dr SHAMOTO, Shin-ichi
Japan Atomic Energy Agency Tokai Research and Development Center
"Nanostructures of Transition Metal Oxides -between Crystal and Amorphous-"

Prof HIROI, Zenji
Tokyo University
"Conductivity and Magnetism of Triangular Lattice Materials with Ni^{3+}"

Dr FURUBAYASHI, Hiroshi
Kanagawa Academy of Science and Technology
"A New Transparent Conductor: Anatase-$Ti_{1-x}Nb_xO_2$"

Prof TAKEDA, Yasuo
Mie University
"Electrochemical Intercalation-disintercalation of Li and Redox Reactions of Transition Elements in Intercalative Materials"

Prof KANNO, Ryoji
Tokyo Institute of Technology
"In-situ Observation of Epitaxial Thin Film Growth and Electrochemical Reactions on Electrode of Lithium Battery"

OBATA, Tuyoshi
NEC Corporation
"Development of Fuel Cell for Portable Devices in NEC"

Prof TAKANO, Mikio
Kyoto University
"Perovskite Fe^{4+} Oxides"

KAWAKAMI, Takateru
Nihon University
"Pressure-induced Antiferromagnetic-ferromagnetic Transition of Fe Perovskite Oxides"

SATO, Ken-ichi
Sumitomo Electric Industries, Ltd.
"Development and Application of Innovative Bi-based Superconducting Wires"

21st Century COE for Kyoto University Alliance for Chemistry "Anglo-German-Japanese Biochemistry Meeting"
Organized by ESAKI, Nobuyoshi; KURIHARA, Tatsuo; AOYAMA, Yasuhiro
5-6 September 2005 (Kyoto, Japan)

Kyoto University COE Program Extension Course "Elements Science in Life and the Future"
Organized by TAKANO, Mikio
1-2 October 2005 (Kyoto, Japan)

Workshop on Nano Scale Beams (NANOBEAM 2005), 36th ICFA Advanced Beam Dynamics Workshop
Organized by NODA, Akira and URAKAWA, Junji
17-21 October 2005 (Kyoto, Japan)

49th Regional Meeting of Japan Society of Clinical Chemistry, Kinki Branch, "Genetic Medicine: Current State and View"
Organized by TANAKA, Seigo
29 October 2005 (Kyoto, Japan)

TANAKA, Seigo
ICR, Kyoto University
"Genetic Analysis of Neurological Disorders and Gene Diagnosis"

GOTO, Susumu
Bioinformatics Center, ICR, Kyoto University
"Genetic Medicine and Bioinformatics"

KAMEDA, Yasushi
Graduate School of Medicine, Osaka University
"Gene Therapy: Current State and View"

Organometallic Seminar XXXIII "A New Trend in Transition-metal-Catalyzed Reactions"
Organized by OZAWA, Fumiyuki
4 November 2005 (Kyoto, Japan)

Workshop on On-Site Small and Medium Scale Neutron Sources
Organized by NODA Akira; KANAYA, Toshiji; IWASHITA, Yoshihisa; SHIMIZU, Hirohiko
18-19 November 2005 (Kyoto, Japan)

Pacifichem 2005 Symposium "Chemical Biology: Small Chemical Compounds as Magic Bullets to Elucidate Biological Mechanisms"
Organized by OSADA, Hiroyuki; UESUGI, Motonari; LIU, Jun O; VERDINE, Gregory L.; SUZUKI, Masaaki; KWON, Ho Jeong
16-17 December 2005 (Honolulu, USA)

INDEX

NAME INDEX

KEYWORD INDEX

Institute for Chemical Research

Kyoto University