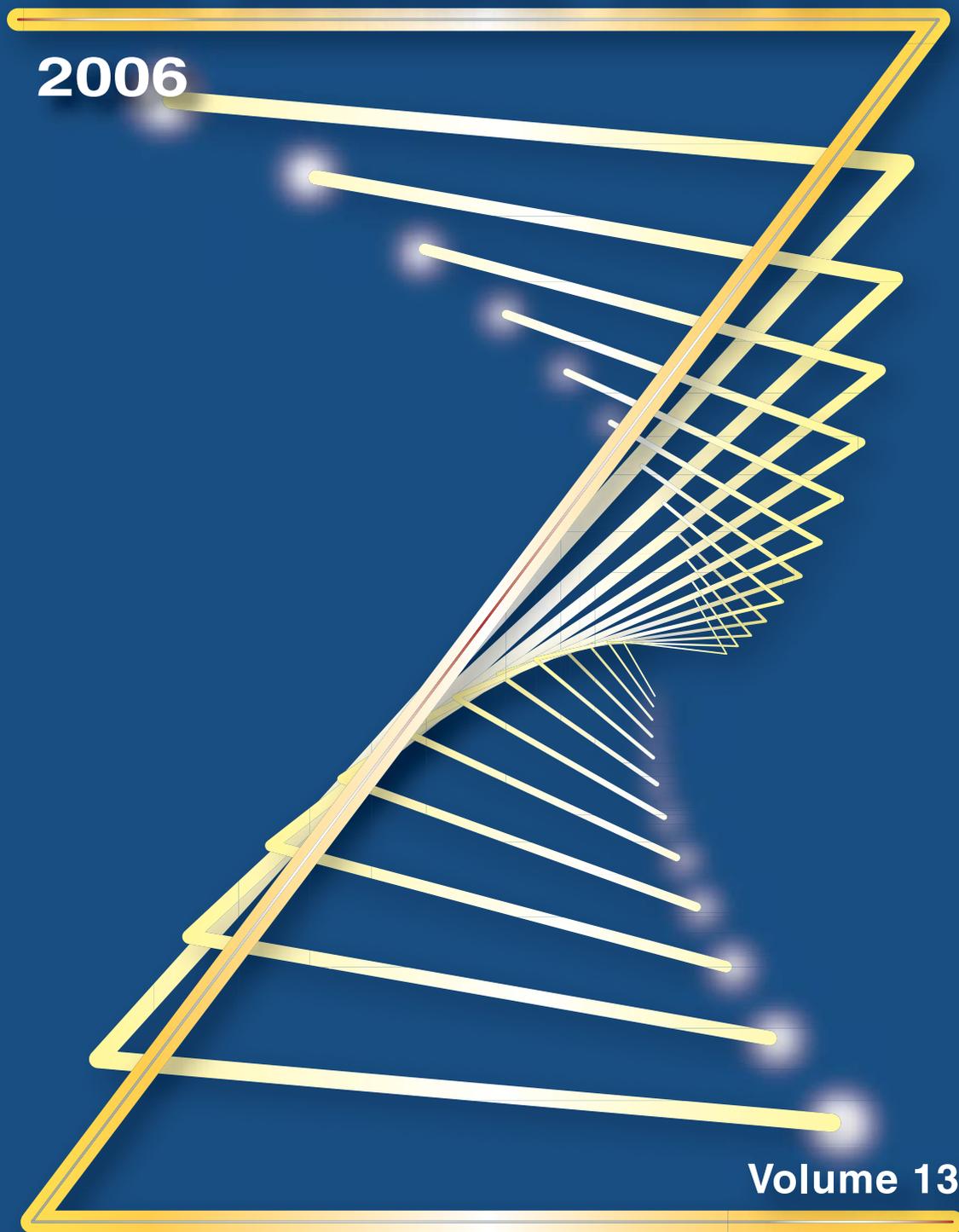


ICR ANNUAL REPORT

2006



Volume 13

Institute for Chemical Research
Kyoto University

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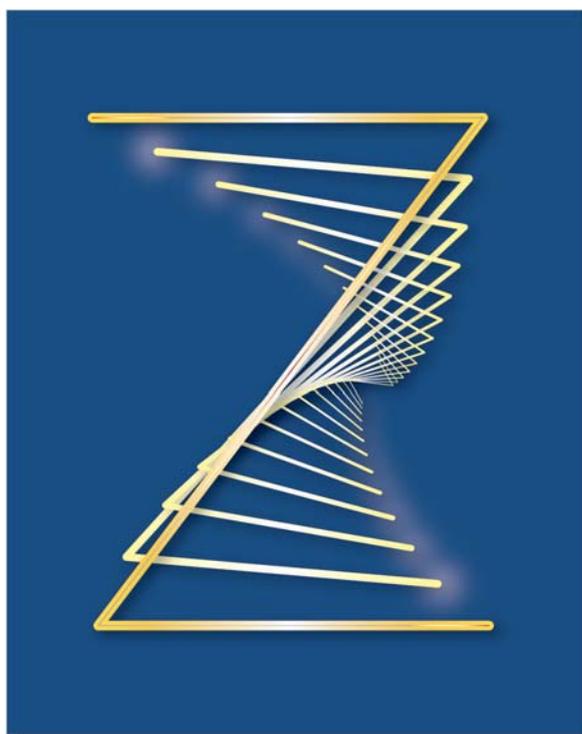
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**ICR
ANNUAL
REPORT
2006**



**Institute for Chemical Research
Kyoto University**
Volume 13



Preface

Institute for Chemical Research (ICR) at Kyoto University was established in 1926 by expanding the Specialized Center for Chemical Research, which was founded in 1915 as part of the Faculty of Science at Kyoto Imperial University. Initially the institute did not possess any full-time faculty members as most of the faculty served concurrently at Kyoto University. Over time, the number of laboratories headed by full-time faculty members as well as the scale of the institute has increased. In 1962, ICR established a graduate school to offer advanced education to graduate students and the research department system was introduced in 1964, which have led to the current ICR organization operated by full-time faculty members.

Our founding vision, “Exploring a basic study on the principle of specific matters in chemistry and further extending its application,” is a legacy that is proudly embraced in today’s ICR. The term “specific matters” refers to groundbreaking and state-of-the-art matters. This statement asserts that ICR entrusts each scientist to choose and pursue research topics in either basic or applied chemistry, and ICR does not restrict research subject matters, but rather encourages open-mindedness and originality. Basics and applications are just like the two sides of a coin, especially since chemistry is comprised of diversified peripheral academic fields. I believe this founding vision truly describes the essence of research activities. A few years ago, the vision and mission of ICR were reexamined and it was determined that the founding vision from 80 years ago appropriately describes the future direction of the chemical research at ICR. Therefore, ICR is actively engaged in this vision and embraces it with absolute confidence.

Although society-sought advanced fields have changed over the years, cutting-edge fields at ICR, which have voluntarily emerged and have achieved excellence in their respective research field, demonstrate the scope of research and the depth of the outcomes from exploring basic chemistry. In this manner, ICR has significantly contributed to society by advancing science and technology in Japan and has earned an excellent reputation at home and overseas. I regard this achievement as the fruits of the diligent efforts and supports of my predecessors.

In 1992, ICR was reorganized. In order to enhance and customize research activities, a new organization was created in April 2004 in concert with the installation of the National University Corporation Kyoto University. To realize ICR’s vision and to answer to social needs, the research objectives were clarified and a new system comprised of five research departments and three research centers was established. Currently, ICR becomes one of the largest university research institutes in the nation as it consists of 31 research fields (laboratories), 104 faculty members, and approximately 240 graduate students. Each laboratory participates in graduate education as a col-

laborative course with one of the seven departments (Science, Engineering, Pharmaceutical Sciences, Agriculture, Medicine, Informatics, and Human/Environmental Studies) and 12 graduate courses. Hence, ICR is fulfilling the mission of a “multi-field collaborative organization” envisioned at its founding 80 years ago.

Developing outstanding young scientists is critical for advancing science and technology. ICR strives to develop open-minded and creative researchers, which only can be achieved in this unique environment. I would like to emphasize a need for collaborative efforts between the university and the research institute in order to realize the most effective education to develop future human resources. Until now, ICR has been a driving force and has served as a leader for the 21st Century Center of Excellence (COE) projects in three major fields: Chemistry, Physics, and the interdisciplinary field of Bioinformatics and Pharmacology. It is my hope that young scientists and graduate students, who are nourished through our international exchange programs and numerous transdisciplinary collaborations, may play a leading role in advancing science and technology not only in Japan, but also throughout the world.

Obviously, the most important task for ICR is to keep producing outstanding research results in chemistry and related fields. However, I strongly believe that ICR should use its uniqueness as a multi-field collaborative organization to work with the graduate school to actively pursue new research themes that cannot be achieved at a graduate school alone. We are currently in the process of establishing a support system for the “Young scientist-led interdisciplinary research projects that envision ICR’s mission.” It is my sincere hope to see this unique seed come to fruition and to carry on our duty as a university research institute.

To embrace our 80th anniversary, we have decided to commission an external review of ICR. Please join me in welcoming Dr. Koji Kaya, Director, RIKEN Discovery Research Institute, who is kindly serving as the chairman of the committee, as well as other members of the external review board. Their straightforward opinions and suggestions on what ICR’s strengths are and how to improve are eagerly awaited. Thus, I am committed to further improving our capacity as a university research institute.

On the occasion of our 80th anniversary, I would like to extend a heartfelt appreciation for your encouragement and support.

January 2007

A handwritten signature in black ink, which appears to read "Esaki Nobuyoshi". The signature is fluid and cursive, written in a professional style.

ESAKI, Nobuyoshi
Director

ICR News 2006

ICR Celebrates 80th Anniversary



■ Chairman of ICR 80th Anniversary Committee:
Prof FUKUDA, Takeshi



Lecture, given by Director Esaki of ICR

Ever since it was formally founded on 4 October 2006 to conduct “fundamental and applied researches on specific subjects in chemistry”, ICR has carried out extensive studies in an extremely wide range of basic and applied chemistry, reaching its 80th anniversary last fall. We celebrated the anniversary on 2 November 2006 by holding Commemorative Lecture Meeting, Ceremony, and Banquet at the Clock Tower Centennial Hall (Centennial Hall and International Conference Hall), Kyoto University. We had another two commemorative events, Poster Exhibition and Historical Exhibition, as separately reported in this Issue.

In the Lecture Meeting, lectures were delivered by Director N. Esaki on the past, present, and future perspective of ICR and by four ICR members, Professors N. Tokitoh, T. Ono, Y. Kanemitsu,

and M. Uesugi on the frontier chemistries under cultivation by these mostly young scientists and their co-workers. The Commemorative Ceremony included an address by Director N. Esaki and greetings by President K. Oike, Kyoto University, Dr. A. Mori (on behalf of Dr. T. Tokunaga), the Ministry of Education, Culture, Sports, Science and Technology, Dr. K. Kaya, RIKEN, and Dr. S. Murai, JST. The Lecture Meeting and Ceremony had an approximate total of 500 participants including some 230 guests from academia and industry. The Banquet was also a success with over 350 participants, getting started with speeches by several guests and proceeding in a friendly and enjoyable atmosphere.



Commemorative Ceremony for 80th Anniversary



Speech by President Oike of Kyoto University



KAGAMIBIRAKI ceremony at the banquet



Address of appreciation from Professor Fukuda

Commemorative Exhibitions:

■ ICR 80th Anniversary Committee:
Prof FUTAKI, Shiroh

Historical Exhibition, “Everlasting Challenge and Innovation”



The Historical Exhibition Room

ICR held its historical exhibition from 3 October to 5 November 2006 at the Historical Exhibition Room in the Clock Tower Centennial Hall to commemorate its 80 years of history. The exhibition named “Everlasting Challenge and Innovation”, showed how scientists at ICR had contributed to the development of science and society. The displays contained “Production of the anti-syphilis drug, Saviol,” “Vinyon, the first man-made fiber in Japan,” “World-leading high-resolution imaging by electron microscopy,” “Fine-powdered iron oxides, from practically demanded size and shape control to nanoscience”, and so on. More than 3800 people visited this exhibition during the term, and pictured the historic scenes from the last 80 years.



A lot of people visited to watch the exhibitions.



Young scientists are interested in the long history of chemical research.

“The Latest Research at ICR”

In addition to the historical exhibition, another exhibition was held at International Conference Hall in the Clock Tower Centennial Hall on 2 November 2006 to introduce current activities of our institute. Together with about 50 panels, slides and movies were employed to introduce researches in each division and laboratory vividly. Samples of research instruments and products were also demonstrated. Intellectual Property Department of Kyoto University had an information booth on the patents applied from our Institute.



Exhibition of the latest research at ICR



Movies introduced the institute’s history, facilities, and research.



Active discussions are held with interesting demonstrations.

CONTENTS

Preface	iii
ICR News 2006	iv
ORGANIZATION	1
TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES	3
Division of Synthetic Chemistry	
Organoelement Chemistry	4
Structural Organic Chemistry	6
Synthetic Organic Chemistry	8
Advanced Inorganic Synthesis	10
Division of Materials Chemistry	
Chemistry of Polymer Materials	12
Polymer Controlled Synthesis	14
Inorganic Photonics Materials	16
Nanospintronics	18
Division of Biochemistry	
Biofunctional Design-Chemistry	20
Chemistry of Molecular Biocatalysts	22
Molecular Biology	24
Chemical Biology	26
Division of Environmental Chemistry	
Molecular Materials Chemistry	28
Hydrospheric Environment Analytical Chemistry	30
Solution and Interface Chemistry	32
Molecular Microbial Science	34
Division of Multidisciplinary Chemistry	
Polymer Materials Science	36
Molecular Rheology	38
Molecular Aggregation Analysis	40
Supramolecular Biology	42
Advanced Research Center for Beam Science	
Particle Beam Science	44
Laser Matter Interaction Science	46
Electron Microscopy and Crystal Chemistry	48
Structural Molecular Biology	50

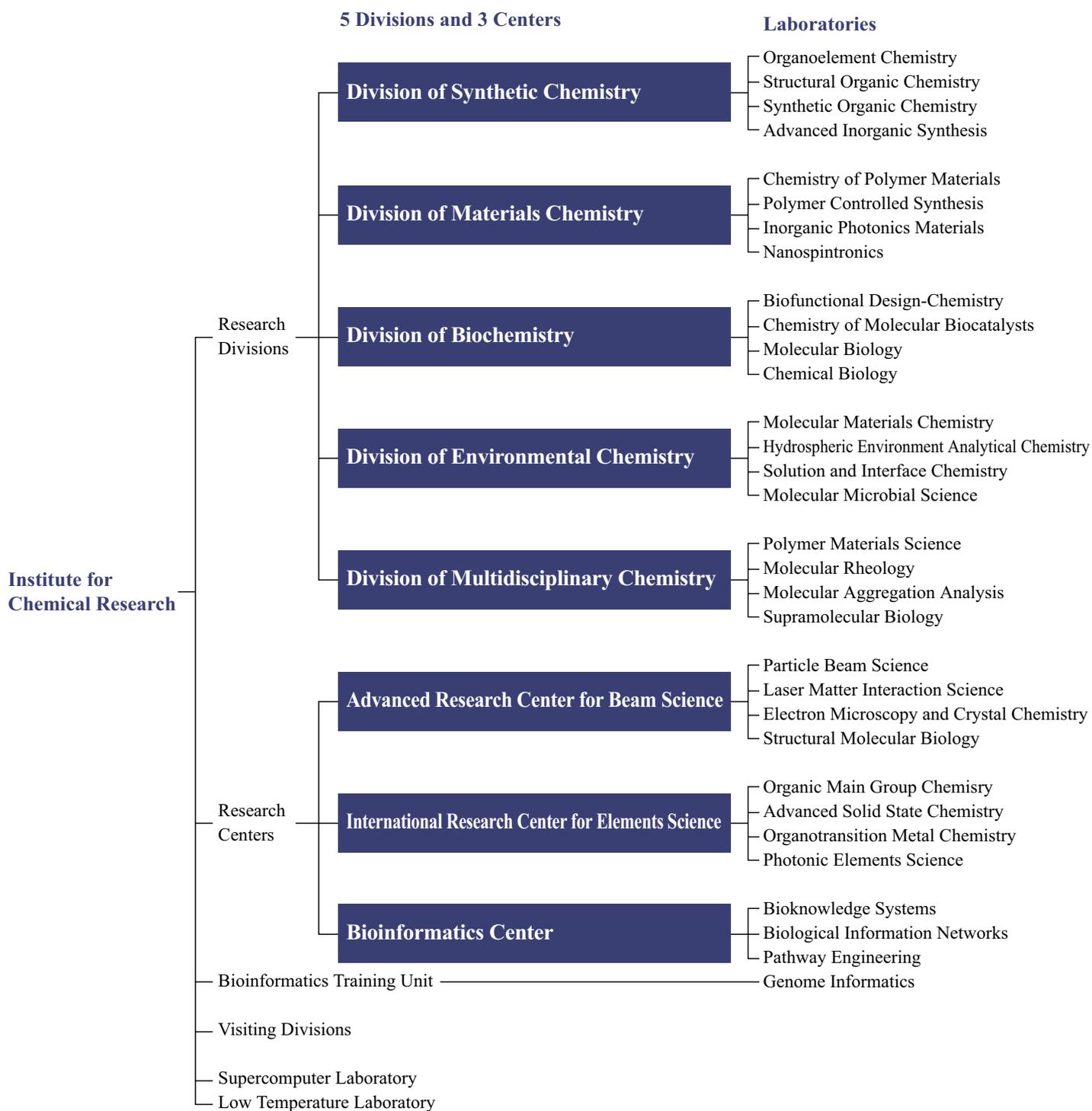
International Research Center for Elements Science	
Organic Main Group Chemistry	52
Advanced Solid State Chemistry	54
Organotransition Metal Chemistry	56
Photonic Elements Science	58
Bioinformatics Center	
Bioknowledge Systems	60
Biological Information Networks	62
Pathway Engineering	64
 Bioinformatics Training Unit	 66
VISITING PROFESSORS' ACTIVITIES IN ICR	69
PERSONAL	73
Retirement	74
Awards	77
Paper Awards	80
Poster Awards	80
Obituary	82
PUBLICATIONS	84
INTERNATIONAL RESEARCH COLLABORATIONS	102
THESES	104
THE 106TH ICR ANNUAL SYMPOSIUM	108
SEMINARS	112
MEETINGS AND SYMPOSIA	116
INDEX	123
NAME INDEX	124
KEYWORD INDEX	127

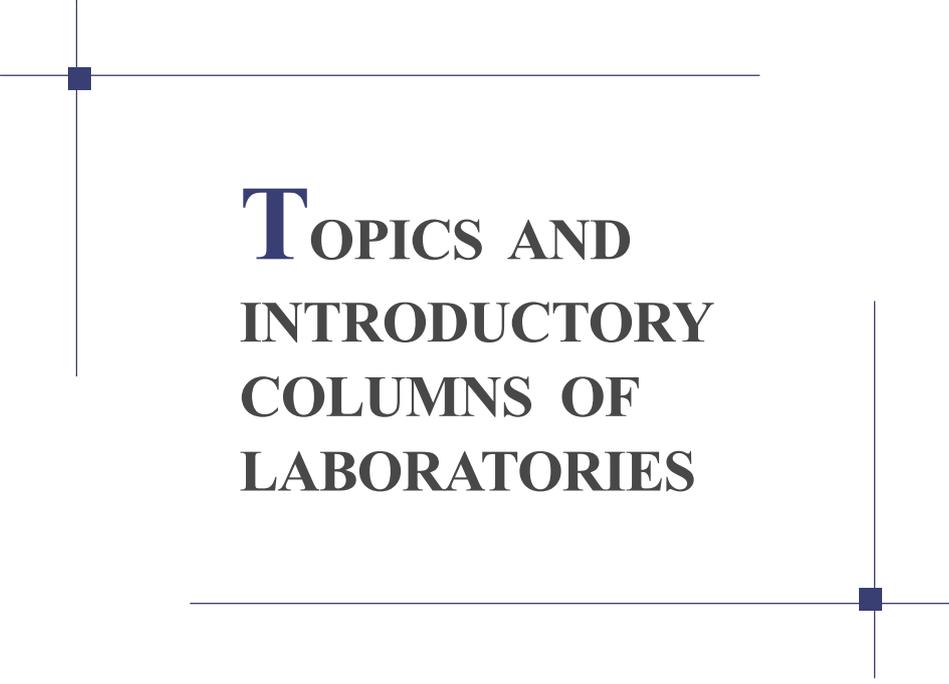
Abbreviations used in the columns

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

A decorative graphic consisting of two horizontal lines and two vertical lines. The top horizontal line starts from the left edge and ends with a small dark blue square. The bottom horizontal line starts from the left edge and ends with a small dark blue square. Two vertical lines extend upwards from the top horizontal line and downwards from the bottom horizontal line, meeting at the top and bottom squares respectively.

ORGANIZATION





TOPICS AND
INTRODUCTORY
COLUMNS OF
LABORATORIES

Division of Synthetic Chemistry - Organoelement Chemistry -

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Prof SCHAUMANN, Ernst
Prof DEVILLANOVA, Francesco A
Technical University of Clausthal, Germany, 29–31 August 2006
Dipartimento di Chimica Inorganica ed Analitica, Università degli Studi di Cagliari, Italy, 3–5 October 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Application of Extremely Bulky Polythioether Ligands to the Synthesis of Novel Transition Metal Complexes Having a Unique Metallacyclic Framework, Tokitoh N, 11th International Symposium on Inorganic Ring Systems (IRIS XI), Oulu, Finland, 30 July– 4 August 2006 (Invited).

Design and Synthesis of Novel Polythioether Ligands Tethered with Extremely Bulky Substituents and Their Application to the Synthesis of Unique Transition Metal Complexes, Tokitoh N, 22nd International Symposium on

the Organic Chemistry of Sulfur (ISOCS-22), Saitama, Japan, 20–25 August 2006 (Invited).

Grants

Tokitoh N, Takeda N, Sasamori T, Nagahora N, 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 Contain-

Synthesis of the Stable “Heavier Alkyne”

Triple-bond compounds between heavier group 14 elements, which are called “*dimetallynes*”, are one of the most fascinating classes of compounds in organometallic chemistry. The chemistry of dimetallynes has been developed in these several years and the syntheses of all symmetrical combinations (Si≡Si, Ge≡Ge, Sn≡Sn, Pb≡Pb) have been achieved by taking advantage of kinetic stabilization using bulky substituents. However, the stable examples of dimetallynes are too limited to elucidate their properties sufficiently. We have succeeded in the synthesis of a new example of a stable germanium analogue, *digermyne* **1**, by using an efficient steric protection group, 2,6-bis[bis(trimethylsilyl)methyl]-4-[tris(trimethylsilyl)methyl]phenyl (Bbt), and revealed its properties. The reaction of dibromodigermyne **2** with KC_8 in benzene resulted in the formation of digermyne **1**. The triple-bond character of **1** was fully examined based on the results of spectroscopic and X-ray crystallographic analyses, and theoretical calculations together with studies

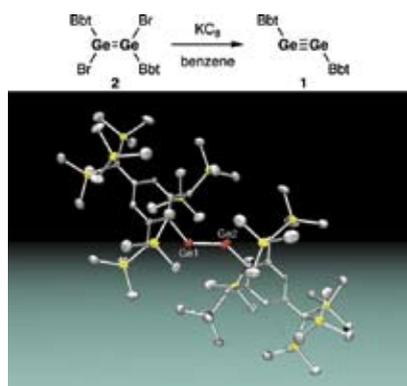


Figure 1. Synthesis of the stable digermyne, **1**, and its structure.

on the reactivities. Digermyne **1** showed a shorter Ge≡Ge bond length than that of the previously reported digermyne, $\text{ArGe}\equiv\text{GeAr}$ (Ar = 2,6-[(*i*-Pr)₂C₆H₃]₂-C₆H₃-).

Synthesis and Applications of a New β -Diketiminato Ligand

The chemistry of β -diketiminato ligands has been extensively studied, and it has been revealed that they can stabilize the metals with unusual valency, such as group 4 metals. In this project, we have studied the synthesis of a new lithium β -diketiminato **3** bearing an extremely bulky substituent, 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl (Tbt) group, and its application toward complexation with group 4 metals. Reactions of **3** with $[\text{MCl}_4(\text{thf})_2]$ (M = Ti, Zr, Hf) gave the corresponding trichlorides **4a-c**. The structures of **4a-c** were definitively determined by X-ray crystallographic analysis. Next, with expectation of obtaining the corresponding low-valent compounds of group 4 metals, the reductions of **4a-c** were attempted. The reactions of **4a-c** with KC_8 in the presence of TMEDA and LiCl resulted in the formation of unexpected imido complexes **5a-c**, respectively.

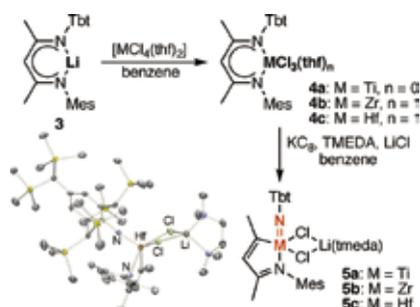


Figure 2. Syntheses of the complexes **4** and **5** and structure of the Hf complex **5c**.

ing 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.

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 2006.

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

Awards

Nagahora N, The Best Oral Presentation Award, The 86th Annual Meeting of the Chemical Society of Japan, May 2006.

Mizuhata Y, The Student Lecture Award, The 86th Annual Meeting of the Chemical Society of Japan, May 2006.

Matsumoto T, The Best Poster Award, 18th Symposium on Fundamental Organic Chemistry, Japan, 9 October 2006.

Nakamura K, Yamanaka R, Matsuda T, Harada T, Tetrahedron: Asymmetry Most Cited Paper 2003–2006 Award, October 2006.

Takeda N, The Society of Synthetic Organic Chemistry, Japan, Kansai Branch Awards, 8 November 2006.

Sasamori T, The ICR Award for Young Scientists, 15 December 2006.

Division of Synthetic Chemistry - Structural Organic Chemistry -

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



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KATO, Keisuke (UG)

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KITAGAWA, Toshikazu (D Eng) Mie University

Visitor

DANQUIGNY, Alain School of Chemistry, University of Southampton, UK, 11 April–10 June 2006

Scope of Research

Fundamental studies are being conducted for creation of new functional materials with novel structures and properties. The major subjects are: organo-chemical transformation of fullerenes C_{60} and C_{70} , specifically organic synthesis of endohedral fullerenes by the technique of molecular surgery; generation of alkylated fullerene cations and their application for the synthesis of functional material; synthesis of new redox-active π -systems.

Research Activities (Year 2006)

Presentations

Synthesis and Properties of Fullerene C_{70} Encapsulating Hydrogen Molecule(s), Murata Y, Maeda S, Murata M, Komatsu K, 209th Meeting of the Electrochemical Society, 10 May 2006, Denver, USA.

Organic Synthesis of Endohedral Fullerenes by Molecular Surgery, Murata Y, 18th Symposium on Fundamental Organic Chemistry, 8 October 2006, Fukuoka, Japan (Invited).

Fine Tuning of the Orifice Size: Synthesis of an Open-cage Fullerene Containing Selenium at the Rim of the Orifice and Insertion of Molecular Hydrogen, Murata Y, Chuang S-C, Komatsu K, The 10th International Kyoto Conference on New Aspects of Organic Chemistry, 16 November 2006, Kyoto, Japan.

Grants

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

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

Murata Y, Academic-Industrial Cooperative Research Fund, April 2006–March 2007.

Awards

Murata Y, Osawa Award, The Fullerenes and Nanotubes Research Society, 8 January 2006.

Murata Y, Young Scientists' Prize, the Commendation for Science and Technology by the MEXT, 18 April 2006.

Murata M, President Prize of Kyoto University, Kyoto University, 20 March 2006.

Synthesis of Selenium-containing Open-cage Fullerene C₆₀

Open-cage fullerene is one of the current synthetic targets of fullerene chemistry besides its well developed exohedral functionalization topic. The ultimate objective for creation of an orifice on the fullerene cage lies in the replacement of conventional methods for the preparation of endohedral compounds and elucidation of their physical and chemical properties. In order to tune the size of the orifice of open-cage fullerenes, we synthesized the selenium-containing open-cage C₆₀ by three-step organic synthesis from fullerene C₆₀. The insertion of molecular hydrogen into the open-cage C₆₀ was achieved in 100% yield under milder conditions compared with those for a sulfur analogue. The kinetic measurements for release of the hydrogen molecule and the X-ray structure analysis revealed that the size of the orifice is larger than that of the sulfur analogue.

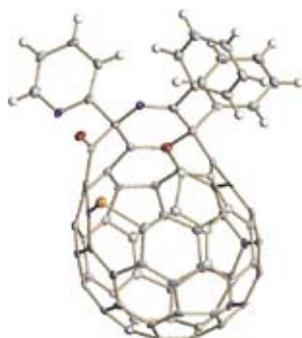


Figure 1. X-ray structure of the selenium-containing open-cage C₆₀.

Encapsulated Hydrogen Molecule as a Sensitive NMR Probe

To examine the effect of encapsulated hydrogen inside C₆₀ upon the reactivity of the outer fullerene cage, the solid-state mechanochemical dimerization of H₂@C₆₀ was conducted. It was found that the dumbbell-shaped dimer, (H₂@C₆₀)₂, was obtained similarly to the reaction of empty C₆₀. Apparently, the inside hydrogen does not affect the reactivity of the outer C₆₀ cage. The ¹H NMR signal for the inside hydrogen was observed as a singlet at $\delta = 4.04$ ppm, which is 8.58 ppm upfield shifted from free hydrogen. Three fullerene derivatives were also synthesized by Bingel reaction, benzyne addition, and Prato reaction in order to further investigate this issue. The NMR signal for encapsulated hydrogen was observed at $\delta = 3.27$ ppm for the Bingel adduct, -4.30 ppm for the benzyne adduct, and -4.64 ppm for the Prato adduct. These upfield shifts are quite similar to those reported for the NMR signal of ³He encapsulated in the corresponding derivatives. Thus, the

inside molecular hydrogen of C₆₀ can also be used as a good probe to investigate the chemical reactions at the exterior of the fullerene cage.

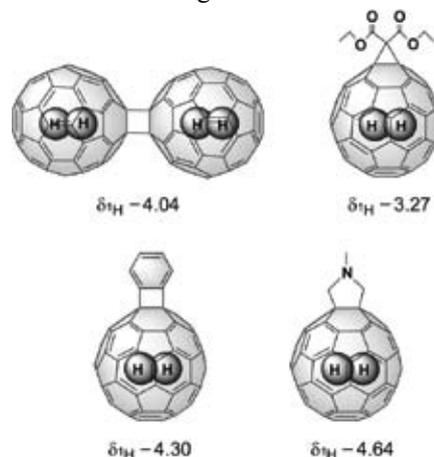


Figure 2. Derivatives of H₂@C₆₀ with the chemical shift of encapsulated hydrogen molecule.

Synthesis of Endohedral Fullerene C₇₀ Encapsulating Hydrogen Molecule(s)

Since the inner space of C₇₀ is larger than that of C₆₀, it might be possible that more than one small molecules be encapsulated. Recently open-cage C₇₀ derivative **1** was synthesized by applying the procedure similar to that used for the synthesis of open-cage C₆₀. Molecular hydrogen was successfully inserted into **1** by treatment with high-pressure hydrogen gas (890 atm) at 200°C. Not only H₂@**1** (97%) but also (H₂)₂@**1** (3%) were found to be formed under these conditions. The complete closure of orifice of H₂@**1** and (H₂)₂@**1** has been achieved via four-step organic reactions without loss of encapsulated hydrogen molecule(s), thus having led to the formation of H₂@C₇₀ and (H₂)₂@C₇₀ for the first time.

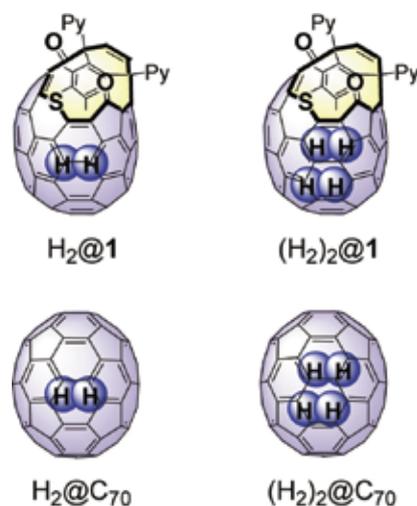


Figure 3. Structures of H₂@**1**, (H₂)₂@**1**, H₂@C₇₀, and (H₂)₂@C₇₀.

Division of Synthetic Chemistry - Synthetic Organic Chemistry -

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URUNO, Yoshiharu (M2)

HAYASHI, Kazuhiro (M1)

SUE, Daisuke (M1)

UYAMA, Makoto (UG)

Visitors

Prof RUANO, Garcia Universidad Autónoma de Madrid, Spain, 21 August 2006

Prof MA, Shengming Shanghai Institute of Organic Chemistry, China, 8 November 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Some Aspects of Asymmetric Synthesis under Environmentally Benign Conditions, Kawabata T, IUPAC Second International Symposium on Green/Sustainable Chemistry, 12 January 2006.

Highly Regioselective Acylation of Sugars by Chiral Nucleophilic Catalysts, Kawabata T, The 8th International Symposium on Organic Reactions, 24 April 2006.

Structural and Functional Investigation of D,L-Oligomers, Kawabata T, International Molecular Chirality Conference (MC 2006), 18 May 2006.

Toward the Development of Chiral 2-Metallabiphenyls, Kawabata T, 7th Tetrahedron Symposium, 26 May 2006.

Direct Regioselective Acylation of Sugars by C_2 -Symmetric Chiral Nucleophilic Catalysts, Muramatsu W,

IUPAC International Conference on Biodiversity and Natural Products (ICOB-5 & ISCNP-25), 24 July 2006.

Regioselective Acylation of Sugars by Nucleophilic Catalysis, Kawabata T, 45th Tutzing Symposium: Organocatalysis, 10 October 2006.

Enolate Chemistry at Room Temperature Using Metal Hydroxides, Moriyama K, The 10th International Kyoto Conference on New Aspects of Organic Chemistry (IKCOC-10), 16 November 2006.

Phenolphthalein-based Chemosensors for Diamines and Unprotected Dipeptides in Water, Tsubaki K, The 3rd Seoul-Kyoto-Osaka Joint Symposium on Pharmaceutical Sciences for Young Scientists, 27 November 2006.

Grants

Kawabata T, Fine Organic Synthesis by Nucleophilic

Regioselective Acylation of Sugars by Nucleophilic Catalysis

Direct regioselective functionalization of multi-functionalized substrates is one of the goals of current research toward the development of advanced molecular transformation for the next generation. We report here a highly regioselective acylation of sugars with chiral nucleophilic catalysts. Treatment of a glucose derivative with 1 mol% of a catalyst and 1.1 mol eq. of isobutyric anhydride in chloroform at -20°C gave the 4-acylated glucose derivative and the 3-acylated surrogate in a 99:1 ratio in 98% yield. The corresponding 6-isomer, 2-isomer, and the di-acylated isomers were not detected at all. The corresponding reaction with 10 mol% of DMAP proceeded in a random way, giving 6-, 4-, 3-, and 2-isomer in a ratio of 38:23:38:1 in a combined yield of 69% together with 19% of the di-acylated isomers and 10% recovery. Thus, discrimination of four hydroxyl groups of the glucose derivative has been achieved by the catalyst through fine dynamic molecular recognition.

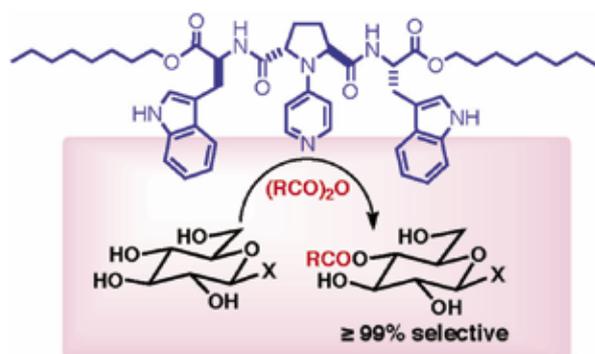
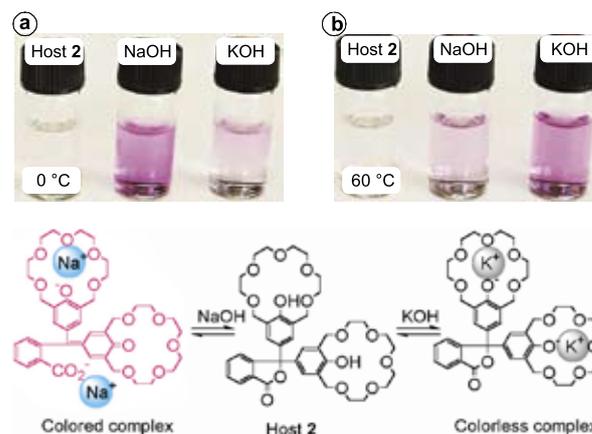


Figure 1. Regioselective Acylation of Sugars with a Nucleophilic Catalyst.

Bidirectional and Colorimetric Recognition of Sodium and Potassium Ions

Host **2** exhibits fascinating and opposite behavior toward sodium and potassium depending on temperature. Coloration caused by the interaction between **2** and NaOH increased as the temperature decreased (a). In contrast, coloration increased as the temperature increased for **2** and KOH (b). The different behaviors for coloration are assumed to be the result from bidirectional complexation. Complexation between **2** and NaOH preferentially gives a colored carboxylate complex, while that between **2** and KOH leads to a colorless complex with a lactone functionality. Why does the colorless complex dominates in the case of **2** and K^+ ? One possible explanation is that potassium ion is strongly inclined to occupy the seat of the *pseudo* phenol 18-crown-6 rings. Occupation of the seat may be favored even with sacrificing the conjugation between two phenol crown rings.



Catalysis, Grant-in-Aid for Scientific Research (A), 1 April 2006–31 March 2009.

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

Tsubaki K, Construction of Molecular Recognition System in Water and Rapid Quantification of Polyamines, Grant-in-Aid for Scientific Research (B), 1 April 2006–31 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.

Awards

Kawabata T, Tetrahedron Letters Most Cited Paper 2003–2006 Award, Elsevier Ltd., 10 September 2006.

Moriyama K, Best Poster Award, The Society of Synthetic Organic Chemistry, Japan, 14 September 2006.

Sue D, Best Poster Award, The Society of Functional Host-Guest Chemistry, Japan, 1 December 2006.

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Scope of Research

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

Research Activities (Year 2006)

Presentations

Magnetic Ferroelectrics Bi,Pb-3d Transition Metal Perovskites: Azuma M, Takata K, Saito T, Shimakawa Y, Takano M, Niitaka S, Belik A A and Ishiwata S, APS March Meeting 2006, Baltimore, USA, 16 March 2006.

Fabrication and Characterization of Multiferroic $\text{Bi}_2\text{NiMnO}_6$ Thin Films: Sakai M, Kan D, Azuma M, Takano M and Shimakawa Y, 67th Autumn Meeting of the Japan Society of Applied Physics, Kusatsu, Japan, 30 August 2006.

Structural Characterization of Epitaxial BaTiO_3 Thin Film by Synchrotron X-Ray Diffraction: Kawai M, Kan D, Sakata O, Kimura S and Shimakawa Y, 67th Autumn Meeting of the Japan Society of Applied Physics, Kusatsu, Japan, 29 August 2006.

Structural Study of SrTiO_3 Showing Room-Temperature Blue Luminescence: Kan D, Masuno A, Shimakawa Y, Sakata O and Kimura S, 67th Autumn Meeting of the Japan Society of Applied Physics, Kusatsu, Japan, 31 August 2006.

Blue-Luminescence from Electron-Doped Metallic SrTiO_3 : Kan D, Ishizumi A, Kanda R, Masuno A, Terashima T, Kanemitsu Y, Takano M and Shimakawa Y, XIII International Workshop on Oxide Electronics, Ischia, Italy, 9 October 2006.

Grants

Shimakawa Y, Synthesis and Structural Characterization of New Functional Transition-Metal Oxides by Solid State Chemistry Approach, Grant-in-Aid for Scientific Research (B), 1 April 2006–31 March 2008.

Shimakawa Y, Invention of Anomalous 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-3d Transition Metal Double Perovskites with Controlled Arrangements of Elements, Natural Sciences Research Assistance, The Asahi Glass Foundation, 1 April 2005–31 March 2007.

Multiferroic Thin Film of $\text{Bi}_2\text{NiMnO}_6$ with Ordered Double-Perovskite Structure

Multiferroic materials, in which ferromagnetic and ferroelectric orders coexist, have attracted lots of attention for technological applications as well as fundamental physics. We have succeeded in fabricating thin films of newly found multiferroic compound $\text{Bi}_2\text{NiMnO}_6$ grown on the SrTiO_3 substrate by pulsed laser deposition. The epitaxially growth and the ordered double-perovskite structure of the thin films are confirmed by X-ray diffraction measurement. Ferromagnetic transition occurred at around 100 K. The observed saturated magnetization at 5 K is $4.2 \mu_B/\text{f.u.}$, which is close to $5 \mu_B/\text{f.u.}$ expected for the ferromagnetic ordering of Ni^{2+} ($S=1$) and Mn^{4+} ($S=3/2$) moments. The clear ferroelectric P-E hysteresis loop was also observed, and the saturated polarization was about $5 \text{ mC}/\text{cm}^2$ above $80 \text{ kV}/\text{cm}$ at 7 K.

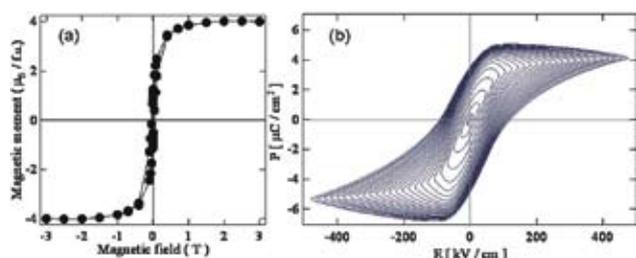


Figure 1. (a) Magnetization curve for $\text{Bi}_2\text{NiMnO}_6$ film measured at 5 K which shows the ferromagnetic ordering of Ni^{2+} and Mn^{4+} moments. (b) Ferroelectric P-E hysteresis curve measured at 7 K.

Half Metallic Ferrimagnet $\text{BiCu}_3\text{Mn}_4\text{O}_{12}$

Considerable attention has been paid to colossal magnetoresistance (CMR). Large MR at a low applied field above room temperature (RT) is highly desirable from practical application point of view.

A cubic ordered perovskite $\text{BiCu}_3\text{Mn}_4\text{O}_{12}$ is a newly found low-field MR compound. This compound is synthesized at a high-pressure of 6 GPa and at 1000°C . $\text{BiCu}_3\text{Mn}_4\text{O}_{12}$ is ferrimagnet below $T_C = 350 \text{ K}$ and its saturated magnetic moment is $10.5 \text{ m}_B/\text{f.u.}$ at 5 K. It shows low resistive metallic behavior. Magnetoresistance (MR) is observed over a wide temperature range below T_C , and the MR below 1T reaches 28% at 5 K. The electronic structure calculation revealed a half-metallic nature of this compound, and the observed large MR under low magnetic field is attributed to spin-polarized tunneling or spin-dependent scattering effects at grain boundaries.

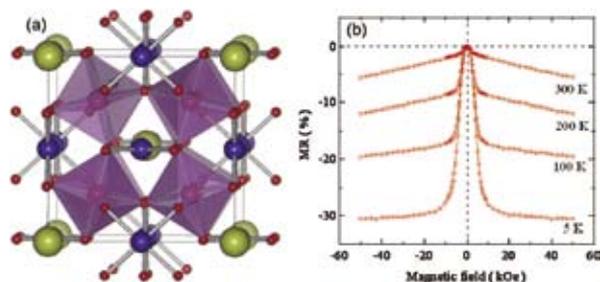


Figure 2. (a) Crystal structure of $\text{BiCu}_3\text{Mn}_4\text{O}_{12}$. (b) Electric resistivity in applied field at 5, 100, 200 and 300 K.

Epitaxial Growth and B-site Cation Ordering in Layered Double Perovskite $\text{La}_2\text{CuSnO}_6$ Thin Films

Epitaxial thin films of layered double perovskite $\text{La}_2\text{CuSnO}_6$ were fabricated on 001-oriented SrTiO_3 , $(\text{LaAlO}_3)_{0.3}-(\text{SrAl}_{0.5}\text{Ta}_{0.5}\text{O}_3)_{0.7}$ (LSAT), and LaAlO_3 substrates with a pulsed laser deposition method. B-site cation ordering of the layer structure can be controlled by tuning the substrate temperature during deposition. X-ray diffraction and scanning transmission electron microscopy revealed that the lattice parameters were strongly correlated with the degree of Cu/Sn ordering. The relationship between the lattice parameters and the B-site cation ordering originates in the orientation of the Jahn-Teller distorted CuO_6 octahedra.

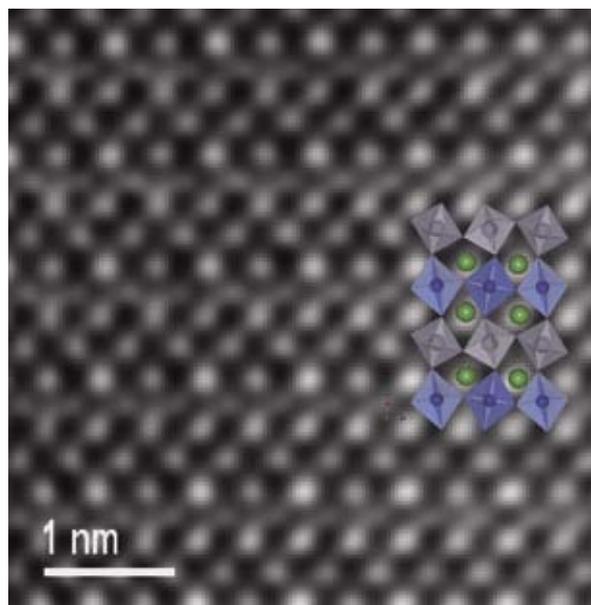


Figure 3. Scanning transmission electron microscope (STEM)-high-angle annular dark-field (HAADF) image of the layered double perovskite LCSO film grown on the LSAT substrate.

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Scope of Research

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

Research Activities (Year 2006)

Presentations

Fukuda T (invited), Surprising New Surface-Science of CPB: 28th Australasian Polymer Symposium, Rotorua, New Zealand, 5–9 February. Society of Rubber Industry Workshop, Uji, 21 April. BASF Asian Workshop on Nanostructured Surfaces, Shanghai, China, 5–11 May. Polymer Symposium, Osaka, 18 May. Tokai Polymer Symposium, Gifu, 25–26 August. 4th IUPAC International Symposium on Radical Polymerization, Lucca, Italy, 3–8 September. Society of Fiber Science and Technology Meeting, Kurashiki, 11 November. Kasenken Symposium, Kyoto, 15 November. Kansai Polymer Symposium, Osaka,

18 November. Riken Symposium, Wako, 28–30 November. Hokuriku Polymer Symposium, Fukui, 8 December.

Tsujii Y (invited), Precise Surface Modification by Surface-initiated LRP: New Technology Presentation Meeting, Tokyo, 27 September.

Ohno K (invited), Hybrid Particles with CPB: Macro Group UK International Conference on Polymer Synthesis, Coventry, UK, 31 July–3 August. Kyushu Polymer Symposium, Kagoshima, 24 November. KIPS Symposium, Kyoto, 1 December.

Goto A (invited), Kinetics of LRP: 55th Spring Meeting, Soc. Polym. Sci., Jpn., Nagoya, 24–26 May.

A New Family of Colloidal Crystals Formed by Suspensions of Silica Particles Grafted with a Concentrated Polymer Brush

A colloidal crystal was newly identified for a liquid suspension of the hybrid particles having a spherical silica core and a shell of well-defined poly (methyl methacrylate) (PMMA) concentrated brush. With increasing particle concentration, the suspension progressed from a (disordered) fluid to a fully crystallized system, going through a narrow crystal/fluid coexisting regime (Figure 1). The crystal had a face-centered-cubic structure with a surprisingly large nearest-neighbor interparticle distance, suggesting that the graft chains, highly extended due to the concentrated brush effect, exerted an interparticle steric potential of that long range. This type of colloidal crystal is new with respect to the origin of long-range interparticle potential and the controllability of many of the system parameters.

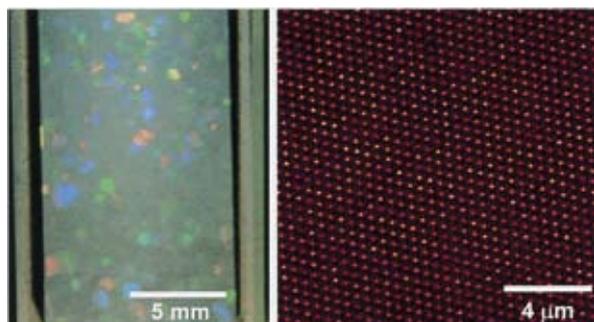


Figure 1. Photograph and confocal laser scanning microscopic image of colloidal crystal.

Ultra-low Frictional Coefficients between Solvent-Swollen Concentrated Polymer Brushes

The interaction forces between surfaces modified with

PMMA brushes were measured in good solvent by atomic force microscopy. The semi-dilute brush ($\sigma = 0.024$ chains nm^{-2} , $M_n = 90,000$, $M_w/M_n = 1.27$) had two different regimes of friction (Figure 2): at low applied loads, the frictional coefficient μ was very low (< 0.001), and in the threshold region, it steeply increased with increasing applied load, approaching the limiting constant value of about 0.1. This transition was ascribed to the interpenetration of the brushes at high loads. Most interestingly, the μ value between concentrated brushes ($\sigma = 0.53$ chains nm^{-2} , $M_n = 88,000$, $M_w/M_n = 1.17$) showed no such transition, staying at low values, lower than 5×10^{-4} , in the whole range of loads studied. This μ value is one of the lowest of all materials and comparable to that achieved for polyelectrolyte semi-dilute brushes with the help of a charge effect. This extremely low frictional property was reasonably ascribed to the fact that swollen concentrated brushes would hardly interpenetrate each other due to the large osmotic pressure and highly stretched chain conformation (entropic interaction).

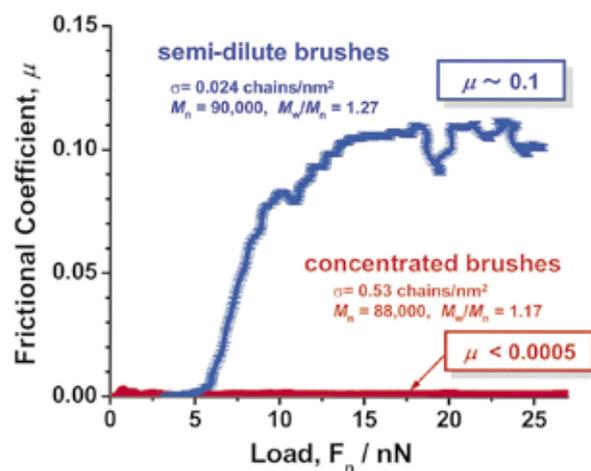


Figure 2. Plot of frictional coefficient μ vs. load for concentrated and semi-dilute PMMA brushes in toluene.

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.

Tsujii Y, Development of Ionic-Liquid Polymer-Based

Electrolyte Membrane by Controlled Graft Polymerization, Strategic Development of PEFC Technologies for Practical Application Program by NEDO, 9 December 2005–20 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.

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Dr CHOW, Tahsin

Dr AMEDURI, Bruno

Prof STUDER, Armido

Prof CRICH, David

Philipps University in Marburg, Germany, 11 September–1 October 2006

National Cheng Kung University, Taiwan, 1 July 2006

Academia Sinica, Taiwan, 27 April 2006

Ecole Nationale Supérieure de Chemie de Montpellier, France, 1 September 2006

Westfälische Wilhelms University, Germany, 23 October 2006

University of Illinois at Chicago, USA, 19 December 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

“Recent Advances in Radical Reactions of Organotellurium Compounds”, Yamago S, 16th IUPAC International Conference on Organic Synthesis, Merida, Mexico, 11–15 June (Invited).

“Effects of Heteroatoms in Highly Controlled Living Radical Polymerizations”, Yamago S, 2nd Pacific Conference on Radical Chemistry, Daejeon, Korea, 5–8 November (Invited).

“Recent Developments in Organotellurium-Mediated Living Radical Polymerization”, Yamago S, 2006 Japan-Taiwan Joint Symposium on Organic Chemistry, Kyoto, Japan, 22–23 April (Invited).

“Electron Microscopy and Diffraction of Radiation-Sensitive Nanostructured Materials”, Schaper AK, Yoshioka T, Ogawa T, Tsuji M, IMC16, The 16th International Microscopy Congress, Sapporo, Japan, 3–8 September,

and other 2 presentations.

“Self-Assembly of Nano-Sized Arrays on Highly Oriented Thin Films of Poly(tetrafluoroethylene)”, Tosaka M, Tsuji M, Kohjiya S, Nagayama K, THERMEC’2006, International Conference on Processing & Manufacturing of Advanced Materials, Vancouver, Canada, 4–8 July (Invited).

Grants

Yamago S, Synthesis of Organic Nano-Molecules by New Living Radical Polymerizations, PRESTO Program, Japan Science and Technology Agency, 1 November 2002–31 March 2006.

Yamago S, Bond Transformation Reactions through Dynamic Interaction of Group 14 Metal-Tellurium Bonds, Grant-in-Aid on Priority Areas, 1 April 2004–31 March 2006.

Highly Efficient Organobismuthine-Promoters for Living Radical Polymerization

The synthesis of functionalized macromolecules with defined structures by living radical polymerization (LRP) is becoming increasingly important since radicals are compatible with a wide variety of polar functional groups, which do not lend themselves to ionic and metal-catalyzed polymerization conditions. While several systems have been developed to conduct LRP, the invention of a new system presents an excellent opportunity to control, with greater precision, molecular structure and to functionalize polymer end-groups. During the course to search more efficient promoters for LRP using organoheteroatom compounds, we found that organobismuthines are most efficient promoters through dual activation mechanisms, namely, thermal generation and degenerative transfer. Both conjugated and unconjugated vinyl monomers are

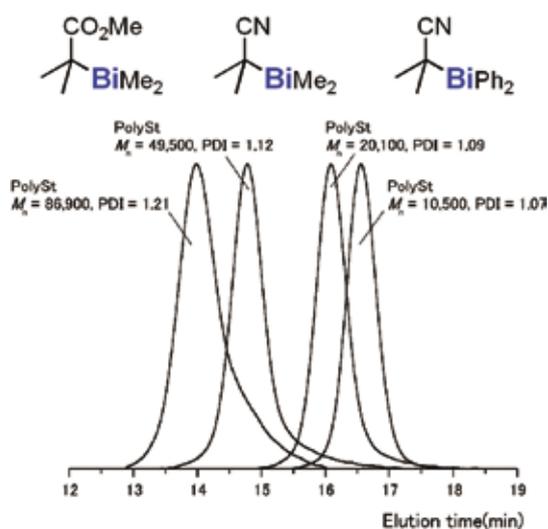


Figure 1. Structures of novel organobismuthine mediators (top) and GPC traces of polystyrene prepared by the mediator and styrene (bottom).

Yamago S, Invention of New Radical Chemistry of “Heavy” Group 15 Heteroatom Compounds, Grant-in-Aid for Scientific Research, (A) (2), 1 April 2005–31 March 2008.

Yamago S, Novel Iterative Synthetic Transformations by Repetitious Uses of Heteroatom Compounds, Grant-in-Aid on Priority Areas, 1 April 2006–31 March 2007.

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

Yamago S, Precision Control of Organotellurium-Mediated Living Radical Polymerization (TERP), Mitsubishi

Foundation Grant, 1 October 2006–30 September 2007.

Dialkylphosphates as New Stereo-Directing Protecting Groups in Oligosaccharide Synthesis

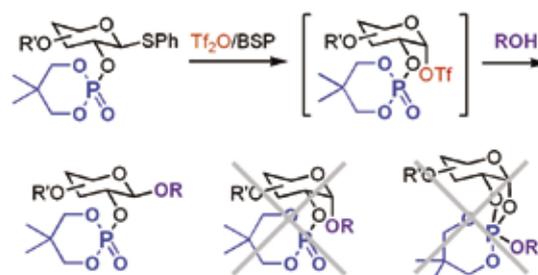


Figure 2. Stereoselective synthesis of 1,2-*trans*-glycoside using C-2 dialkylphosphate protected thioglycosides.

Stereoselective formation of a glycosidic linkage is one of the most important tasks in synthetic carbohydrate chemistry, because the structure of glycosides plays crucial role in many of important biological processes involving oligosaccharides. To date, 1,2-*trans*-glycosides have been prepared so far by intramolecular neighboring group participation of the C-2-acyl protective groups, but this method has serious drawbacks due to the formation of an orthoester side product. We found that dialkylphosphates served as excellent stereo-directing groups for 1,2-*trans*-glycoside synthesis. As the phosphates can be removed after glycosylation, they can be used as stereo-directing protective groups. In addition to this, we found that these protective groups can be used in the iterative glycosylation reactions. Therefore, a variety of oligosaccharides that possess the 1,2-*trans*-glycosidic linkage can be synthesized under a set of glycosylation conditions.

Foundation Grant, 1 October 2006–30 September 2007.

Yamago S, Creation of Functional Organic Materials by Organobismuthine-Mediated Living Radical Polymerization, Industry-University Joint Research for Innovative Seeds Program, Japan Science and Technology Agency, 1 September 2006–31 August 2007.

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.

Tosaka M, Dissipative Structures Induced by Oriented Polymer Thin Films, Tokuyama Science Foundation Grant, 10 May 2006–31 May 2007.

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YAMAMOTO, Hideaki (M1)
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Prof HIMANSHU, Jain Lehigh University, USA, 25–26 July 2006
Prof MCNAMARA, Pam University of Sydney, Australia, 16 October 2006

Scope of Research

In this laboratory, amorphous and polycrystalline inorganic materials and organic-inorganic hybrid low-melting glassy 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-resolution NMR, thermal analysis, various laser spectroscopies and ab initio molecular orbital calculations, and the properties are fully characterized.

Research Activities (Year 2006)

Presentations

Preparation and Application of Organic-inorganic Hybrid Low-melting Glass, Yoko T, Kyushu Synchrotron Photon Factory Completion Memory Symposium, Saga, 25 January 2006 (Invited).

Preparation and Properties of Novel Organic-inorganic Hybrid Low-melting Glasses, Mizuno M, Kakiuchida H, Tokuda Y, Takahashi M, Yoko T, HNM 2006 in Nagaoka, 4–5 February 2006 (Invited).

Preparation and Properties of Novel Organic-inorganic Hybrid Low-melting Glasses by a Non-aqueous Acid-base Reaction Method, Mizuno M, Tokuda Y, Takahashi M, Yoko T, International Symposium on Non Oxide and New Optical Glasses (ISNOG 2006), 10–14 April 2006, Bangalore, India (Invited).

Formation of Self-organized Ordered Micro Structures in Oxide Films through Photo-polymerization Induced Phase Separation, Takahashi M, Maeda T, Tokuda Y, Yoko T, IUMRS-ICA, Cheju, Korea, 16 September 2006.

Organic-inorganic Hybrid Materials through Solventless Processes, Takahashi M, Yoko T, The Ceramics Society of Japan Fall Meeting, Yamanashi, Japan, 19 September 2006 (Invited).

Organically-modified Silicophosphate Materials Prepared by Acid-base Reaction, Takahashi M, Yoko T, The Ceramics Society of Japan Fall Meeting, Yamanashi, Japan, 21 September 2006 (Invited).

Organically-modified Silicophosphate Hybrid Materials Prepared through Acid-base Concept, Takahashi M, Mizuno M, Tokuda Y, Yoko T, The XI International Conference on the Physics of Non-crystalline Solids, Rhodes, Greek, 2 November 2006.

Grants

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.

New Families of Organic-inorganic Hybrid Materials through Solventless Processes

Development of highly functional and reliable materials for optical information processing devices is one of the most important research targets these days. We have been reporting new families of organic-inorganic hybrid materials for such application prepared through solventless condensation processes, by which a flexible structural control at a molecular level is possible. For such purpose, we are working on the solventless condensation between the starting reagents through acid-base reaction and alcohol condensation. The obtained materials are characterized by a unique oxide alternating copolymer structure, enabling us to control the molecular structure for the molecular engineering precisely. Highly transparent and, if necessarily, patternable materials were obtained by these methods, and most of them were found to be suitable for photonics applications. Organically-modified silicophosphate glasses obtained through the acid-base reaction are found to be much better solvent for metal ions and ionic organic chromophores than good organic solvent for them. It is expected for this materials that the figure-of-merit is improved and the device dimension could be largely reduced. The Au-nano particle- and rhodamine 6G-codoped phenyl-modified silicophosphate materials with 100% condensation yield, exhibited a large coefficient of two photon absorption which was 100 times as large as that of Au-nano particle-undoped one. In a case of alcohol condensation in solventless process, we have reported the organically-modified curable siloxane with extremely low optical attenuation, < 0.3 dB/cm, in the telecom window. Figure 1 is a sub-micrometer scale photonic structure obtained by the soft lithography using the present material.

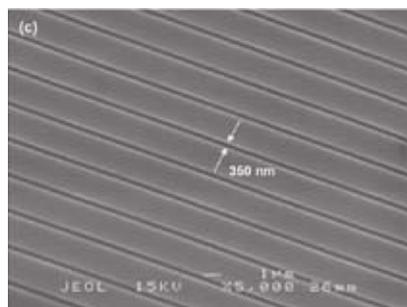


Figure 1. SEM image of photonic structure made of organically-modified siloxane materials obtained by solventless alcohol condensation of vinyltriisopropoxysilane and diphenylsilanediol.

Takahashi M, Inhomogeneous Structures in the Glasses, Grant-in-Aid for Scientific Research for Encouragement of Young Scientists (A), 1 April 2004–30 September 2006.

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

Inverse Methods for the MQMAS NMR Spectral Analysis

A number of structural studies on inorganic glass using experimental and simulation methods have been carried out. This type of study is important because the knowledge of the glass structure leads to an understanding of its physical and chemical properties. MAS NMR is one of the powerful tools to provide the structure information especially on dipolar nuclei ($I = 1/2$). Unfortunately, quadrupolar nuclei ($I \geq 3/2$) provide too broad MAS NMR spectra to be analyzed quantitatively, although half elements have quadrupolar spin. For a better understanding of quadrupolar nuclei in solid state material, Fridman et al. developed MQMAS NMR to provide narrow spectra of quadrupolar nuclei. However, MQMAS NMR lacks quantitative information on the nuclei because the efficiency of multi-quantum spin transition depends on the quadrupolar coupling constant.

In this work, we will provide a direct investigation of the local structure in inorganic glass based both on MQMAS NMR and inverse analysis. An observed spectrum and an inherent distribution of structure parameter, R , are related with each other by

$$I(\varpi) = \int I_0(\varpi; R) \Pi(R) dR \quad (1)$$

where $I(\varpi)$, $I_0(\varpi; R)$, $\Pi(R)$ are the observed spectrum, a theoretical spectrum for R , the distribution of R , respectively. Using equation (1), $\Pi(R)$ can be calculated based on the numerical approach with Tikhonov regularization (inverse analysis). We are now trying to establish inverse analysis to extract the inherent structure distribution in inorganic glass from the measured NMR spectra.

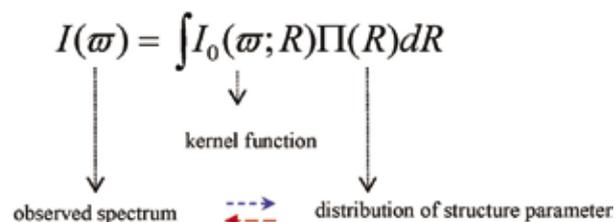


Figure 2. Inverse method for quantitative analysis on MQMAS NMR spectra. The arrows, \leftarrow and \rightarrow , mean direct and inverse problem, respectively. The kernel function can be calculated theoretically using quantum theory.

April 2005–31 March 2006.

Tokuda Y, Fabrication of Pb-free Sealing Glass, JST, Research for Promoting Technological Seeds, 13 September 2006–28 February 2007.

Division of Materials Chemistry - Nanospintronics -

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



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Université Paris-sud, France, 30 May–31 August 2006

University of Tokyo, Japan, 30 November 2006

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 2006)

Presentations

Li₀-FePt Nanoparticles Synthesized via SiO₂-nanoreactor Method, Ono T, 10th MORIS, 6–8 June 2006, Tomiura, Chiba, Japan.

Mesoscopic Fano Effect in Quantum Hybrid Systems, Kobayashi K, Vietnam 2006: 6th Rencontres du Vietnam “Nanophysics: from Fundamentals to Applications”, 8 August 2006, Hanoi, Vietnam.

Excitation of Nano-spin-structure by Spin-polarized Current, Ono T, International Conference on Magnetism, 20–25 August 2006, Kyoto, Japan.

Magnetic Ratchet Effect in Submicron Magnetic Wires with Asymmetric Notches, Himeno A, Kasai S, and Ono T, Gordon Research Conferences (Magnetic Nanostructures), 3–8 September 2006, Oxford, UK.

Excitation of Spin-structure in Nano-magnet by Electrical Current, Ono T, 378th International Wilhelm and Else Heraeus Seminar –Spin Torque in Magnetic Nanostructures–, 22–26 October 2006, Rhöndorf, Germany.

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.

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

Himeno A, Best Poster Award at the 17th International Conference on Magnetism (ICM), August 20–25 2006, Kyoto, Japan.

Resonant Excitation of the Magnetic Vortex Core

Manipulation of the magnetization by spin currents is a key technology for future spintronics. Underlying physics is that spin currents can apply a torque on the magnetic moment when the spin direction of the conduction electrons has a relative angle to the local magnetic moment. This can be generalized to the idea that any kind of spin structure with spatial variation can be excited by a spin-polarized current in a ferromagnet.

A typical example of such a non-collinear spin structure is a curling magnetic structure (magnetic vortex), which appears in a ferromagnetic circular dot. Here we demonstrate that a magnetic vortex core can be resonantly excited by an AC current through a ferromagnetic circular dot when the current frequency is tuned to the eigenfrequency originating from a confinement of a vortex core in a dot. Our micromagnetic simulations with the spin-transfer effect reveal the detailed motion during the excitation; an excited vortex core draws a spiral trajectory to settle in a steady orbital around the dot centre. We succeeded in detecting the predicted resonance by resistance measurements. We found the efficient excitation by an electric current due to the resonance nature and the tunability of the resonance frequency by dot shape, which opens up the potentiality of a simple magnetic dot as a building block for spintronic devices and a rotary actuator for nano-mechanical systems.

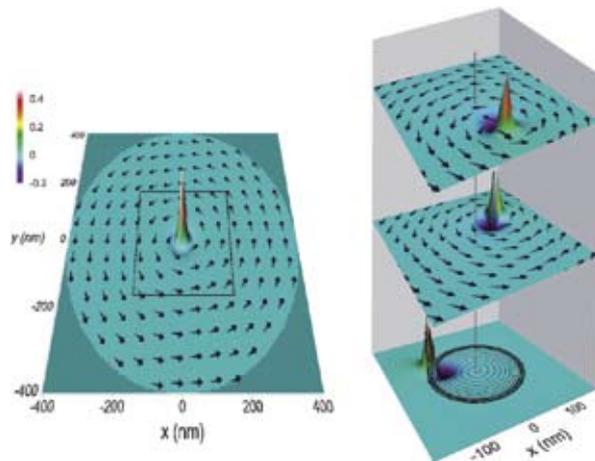


Figure 1. Time evolution of the vortex under the AC current application. Magnetization direction $\mathbf{m} = (m_x, m_y, m_z)$ inside the dot on the xy plane was obtained by micromagnetic simulation. The 3D plots indicate m_z with the $m_x - m_y$ vector plots superimposed. The plot on the left represents the initial state of the vortex core situated at the center of the dot with $r = 410$ nm. The 3D plots on the right show the vortex on the steady orbital at $t = 80.6, 81.5,$ and 82.3 ns after applying the AC current.

Spin Injection into the Superconductor

The efficient spin injection, accumulation and transport in solid state devices are the central issue in both fundamental and technological points of view. In general, the spin polarized electrons injected from the ferromagnets (F) into the nonmagnetic materials (N) such as normal metals, semiconductors, and superconductors (SC) create nonequilibrium spin accumulation in N . The spin accumulation plays an important role in the field of spintronics which will be realized by manipulating the spin degree of freedom of electrons.

Recently it was reported that a spin accumulation signal was detected in a lateral $\text{Ni}_{80}\text{Fe}_{20}/\text{Cu}/\text{Ni}_{80}\text{Fe}_{20}$ spin valve device by using a non-local spin transport measurement. However, the possible spin accumulation in SC 's still remained to be explored, which is stimulating because the strong competition between superconductivity and magnetism is induced by artificial spin polarization in SC 's. Theoretically, the non-local spin signal is greatly enhanced when N falls into the superconducting state below its transition temperature (T_C). This enhancement is due to the fact that SC is a low-carrier system for spin transport but not for charge transport.

We addressed the issue by using the tunnel-junction $F/SC/F$ spin valve structure with the non-local measurement technique. By injecting an appropriate current, the spin signal was observed to be several times larger in the superconducting state than in the normal state, consistent with the theoretical prediction.

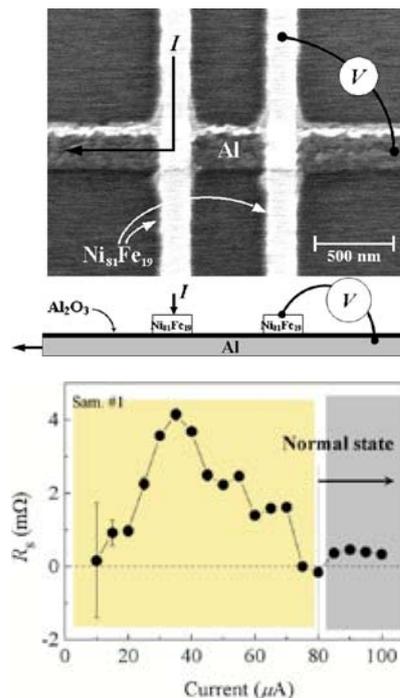


Figure 2. (Top) Scanning electron microscope image of a lateral spin valve device, with the geometry of the non-local measurement. (Bottom) Device cross-section.

Figure 3. Current dependence of the non-local spin accumulation signal R_S at the superconducting state (at low current regime), showing the enhancement of the spin signal compared to that at the normal state (at high current regime).

Division of Biochemistry - Biofunctional Design-Chemistry -

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Visitors

Dr ARWYN, Tomos Jones	Welsh School of Pharmacy, Cardiff University, UK, 13–15 July 2006
Mr BANOCZI, Zoltan	Hungarian Academy of Sciences, Hungary, 23 July–5 August 2006
Prof MATILE, Stefan	University of Geneva, Switzerland, 3 August 2006
Dr SAKAI, Naomi	University of Geneva, Switzerland, 3 August 2006
Prof WOOLLEY, Andrew	University of Toronto, Canada, 3–9 August 2006
Prof GARIEPY, Jean	University of Toronto, Canada, 3–9 August 2006

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 2006)

Presentations

“Membrane-permeable Arginine-rich Peptides and the Interaction with Cell Membranes”, Futaki S, 10th Naples Workshop on Bioactive Peptides, Naples, Italy, 11–14 June.

“Oligoarginine Vectors for Intracellular Delivery: Design and Cellular-uptake Mechanisms”, Futaki S, The First FIP-APSTJ Joint Workshop on Gene Delivery, Sapporo, 10–12 July.

“Transmission of Extramembrane Conformational Switch into Channel Current; Design and Construction of Artificial Metal-gated Receptor Channel”, Kiwada T, Sonomura K, Sugiura Y, Asami K, and Futaki S, International Conference of 43rd Japanese Peptide Symposium/4th Peptide Engineering Meeting, Yokohama, 5–8

November.

“Arginine-rich Peptides and the Internalization Mechanisms”, Futaki S, International Mini Symposium Membrane-permeable Peptides: Chemistry, Biology and Therapeutic Applications, Kyoto, 10–11 November.

“Artificial Ion Channels Gating by Extramembrane Conformation Switch”, Futaki S, Japan-Italy Research Cooperative Program: Japan-Italy Symposium of New Trends in Enzyme Science and Technology, Nagoya, 15–17 November.

“Creation and Applications of Artificial Zinc Finger-type DNA Binding Proteins”, Imanishi M, 55th Annual Meeting, The Japan Society for Analytical Chemistry, Toyonaka, 22 September.

“Selective Modification of N-glycosides of Transferrin

Transmission of Extramembrane Conformational Switch into Channel Current; Design and Construction of Artificial Metal-gated Receptor Channel

Ion channels and receptors are among the most biologically important classes of membrane proteins that transmit outside stimuli into cells. The creation of artificial proteins with these functions is a challenge in peptide/protein engineering in view of the creation of novel functional nano-devices as well as understanding the biological machinery. We have developed a novel Fe(III)-gated ion channel system that is comprised of assemblies of a channel forming peptide alamethicin bearing an extramembrane segment. The extramembrane segment contains a pair of diiminoacetic acid derivatives of lysine (Ida) residues. Interaction with Fe(III) induces the structural alternation of the extramembrane segment via the chelate formation with Ida residues, which eventually leads to an increased channel current (ion influx). This result exemplifies the feasibility of utilizing the conformational switch of the extramembrane segment for the current control in artificial channel systems, a concept that can be applicable for the design of various artificial receptor ion channel systems.

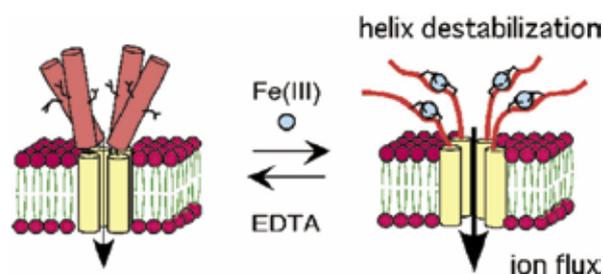


Figure 1. Schematic representation of the artificial receptor channel that transmits outside stimuli (metal) to inside the membrane as an increase in the ion flux.

Direct and Rapid Cytosolic Delivery Using Cell-penetrating Peptides Mediated by Pyrenebutyrate

Intracellular delivery of bioactive molecules using arginine-rich peptides, including oligoarginine and HIV-1 Tat peptides, is a recently developed technology. We found a dramatic change in the methods of internalization for these peptides brought about by the presence of pyrenebutyrate, a counteranion bearing an aromatic hydrophobic moiety. In the absence of pyrenebutyrate, endocytosis plays a major role in cellular uptake. However, the addition of pyrenebutyrate results in direct membrane translocation of the peptides yielding diffuse cytosolic peptide distribution within a few minutes. Using this method, rapid and efficient cytosolic delivery of the enhanced green fluorescent protein (EGFP) was achieved in cells including rat hippocampal primary cultured neurons. Enhancement of bioactivity on the administration of an apoptosis-inducing peptide is also demonstrated. Thus, coupling arginine-rich peptides with this hydrophobic anion dramatically improved their ability to translocate cellular membranes, suggesting the great impact of this approach on exploring and controlling cell function.

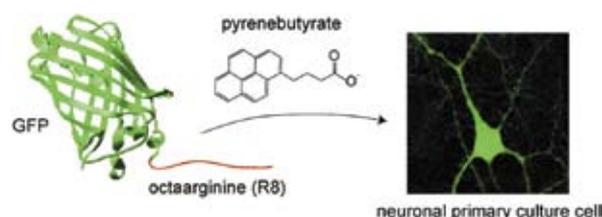


Figure 2. Counteranion-based direct and rapid translocation of R8-conjugated enhanced green fluorescent protein (EGFP) into primary culture cells.

with Therapeutic Drugs for the Receptor Targeting”, Nakase I, The First FIP-APSTJ Joint Workshop on Gene Delivery, Sapporo, 10–12 July.

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, Cell Targeting Delivery Peptides: Functional Elucidation and Delivery Control, SORST Program, Japan Science and Technology Agency, 1 April 2006–31 March 2008.

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.

Nakase I, Design and Synthesis of New Carrier Peptides Having Functions of Recognition toward Both Proteoglycans and Cellular Markers for Efficient Delivery of Therapeutic Agents into Cells, Grant-in-Aid for Young Scientists (Start Up), 1 April 2006–31 March 2008.

Award

Nakase I, The Best Presentation Award, The First FIP-APSTJ Joint Workshop on Gene Delivery, Sapporo, 24 July 2006.

Division of Biochemistry - Chemistry of Molecular Biocatalysts -

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Scope of Research

Our research covers the comprehensive understanding of the physiological roles of biocatalysts (enzymes) as well as the reaction mechanism and specificity of each enzyme. 1) Studies on diglycosidases 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) Directed evolutionary studies of *Pseudomonas* lipase. 5) Studies on the activation/inactivation process of plant hormones. 6) Molecular mechanism of regulation of phenylpropanoid pathway in plants.

Research Activities (Year 2006)

Presentations

Inhibitors of IAA-Amino Acid Conjugate Synthetases and Hydrolases as Chemical Probes to Study IAA Homeostasis, Tai LH, Hiratake J, Shimizu B, Mizutani M, Sakata K, 11th IUPAC International Congress of Pesticide Chemistry, Kobe, 8 August.

X-ray Crystallography of a Diglycosidase from Plants, Saino H, Mizutani M, Hiratake J, Shimizu T, Kato H, Sakata K, 2006 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 27 March.

Glucosylation of Scopoletin in *Arabidopsis* Roots, Kai K, Shimizu B, Yamaguchi H, Mizutani M, Sakata K, 2006 Annual Meeting, Jpn. Soc. Plant Physiol., 20 March.

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.

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.

Design, Synthesis and Evaluation of γ -Glutamyl Transpeptidase Inhibitors

γ -Glutamyl transpeptidase (GGT) catalyzes the hydrolysis of glutathione and its *S*-conjugates and plays a pivotal role in glutathione metabolism. GGT is involved in important biological events such as drug resistance and metastasis of cancer cells by detoxification of xenobiotics and reactive oxygen species, and is also implicated in physiological disorders such as Parkinson's disease, cardiovascular diseases and asthma through glutathione metabolism and leukotriene biosynthesis. We designed and synthesized a series of γ -phosphono diester glutamate analogues as mechanism-based inhibitors of GGT. The phosphonates reacted with the N-terminal catalytic Thr residue of GGT to cause facile enzyme inactivation. A series of the phosphonate inhibitors were synthesized to probe successfully the active-site geometry of human GGT, where a specific residue in the Cys-Gly binding site played a critical role in recognizing the C-terminal carboxy group of glutathione and its conjugates. The phosphonate diesters were highly selective towards GGT and did not inhibit glutamine amidotransferases, the important enzymes for purine and pyrimidine biosynthesis. The phosphonate diester-based GGT inhibitors serve as drug leads and biological probes that gain insight into the hitherto undefined physiological roles of GGT and the relationships between GGT and a variety of diseases.

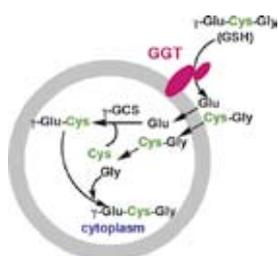


Figure 1. Physiological role of GGT.

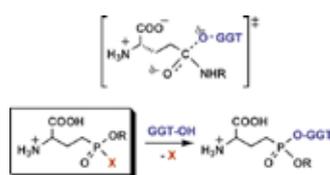


Figure 2. Proposed transition state of the reaction catalyzed by GGT and γ -phosphono diester glutamate analogues as mechanism-based inhibitors of GGT.

Chemical Inhibitors for Abscisic Acid Catabolism

A plant hormone, abscisic acid (ABA), regulates many important physiological processes including adaptive responses to abiotic stresses. The main catabolic pathways involve hydroxylation of the C-8' position of ABA by cytochrome P450 monooxygenases (P450), and we recently identified CYP707As as ABA 8'-hydroxylase. Plant growth retardants (PGRs) are known to reduce the shoot growth of plants by inhibiting P450s in gibberellin biosynthesis. We performed detailed analyses of the inhibitory effects of PGRs on *Arabidopsis* ABA 8'-hydroxylase. Uniconazole-P was found to be a strong competitive inhibitor ($K_i = 8.0$ nM) of ABA 8'-hydroxylase. Uniconazole-P-treated *Arabidopsis* plants showed enhanced drought tolerance (Figure 3). In uniconazole-P-treated plants, endogenous ABA levels increased 2-fold as compared with the control. Thus, specific inhibitors of ABA catabolism can manipulate ABA homeostasis in plants and are potentially very useful tools for cellular and molecular investigations in the field of plant physiology as well as for potential agricultural chemicals.

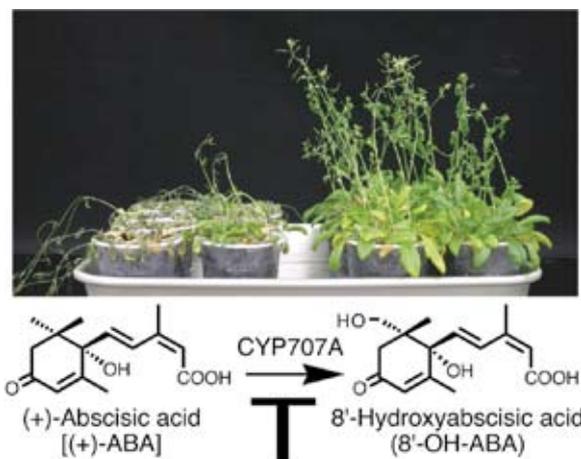


Figure 3. Inhibitors for ABA catabolism can manipulate ABA homeostasis and enhance plant drought tolerance.

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

Awards

Mizutani M, The JSCR Award for the Encouragement of Young Scientists, "Biochemical Studies on Cytochrome P450 Monooxygenases in Abscisic Acid and Plant Steroid Metabolism", The Japanese Society for Chemical Regulation of Plants, 30 October 2006.

Ohnishi T, Poster Award, "Functional Characterization of *Arabidopsis* CYP90C1 and CYP90D1 Encoding Brassinosteroids C-23 Hydroxylases". 8th International Symposium on Cytochrome P450 Biodiversity and Biotechnology, Swansea, UK, 27 July 2006.

Ohnishi T, Poster Award, "Biochemical Characterization of Brassinosteroid C-3 Oxidase", The 41th Annual Meeting of the Japanese Society for Chemical Regulation of Plants, Osaka, Japan, 30 October 2006.

Division of Biochemistry - Molecular Biology -

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Mr LI, Linchuan

Dr HWANG, Ildoo

Dr CHO, Hyung-Taeg

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College of Life Science, Peking University, China, 2–17 August 2006

College of Life Science, Peking University, China, 7 August–7 October 2006

College of Life Science, Peking University, China, 7 August–7 October 2006

Pohang University of Science and Technology, Korea, 26–27 May 2006

Chungnum National University, Korea, 26–27 May 2006

Dong-A University, Korea, 26–27 May 2006

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. The current major subjects are the two-component response regulators involved in cytokinin signaling, HD-Zip proteins and phosphatidylinositol 4-phosphate 5-kinases required for phospholipid signaling, COP9 signalosome modulating protein degradation, and cyclins and CDKs controlling cell cycle.

Research Activities (Year 2006)

Presentations

Signal Transduction Regulating Morphological Differentiation of Plant Cells, Aoyama T, Symposium: A New Line in the Study of Plant Totipotency, 28 January (Nagoya).

Plant Morphogenesis Responding to Environmental Stimuli, Tsuge T, COE Seminar: Chemicalbiology Mini-Symposium, 15–16 March (Kyoto).

COP9 Signalosome: The Key Modulator of Signal Transduction in Plants and Animals, Tsuge T, International

Symposium on Biotechnological Approaches for Agriculture and Medicine, 2 November (Busan, Korea).

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 2004–31 March 2007.

A Key Regulator of Ploidy Levels in Endoreduplication of *Arabidopsis thaliana*

Eukaryotic cells generally proliferate through the mitotic cell cycle, which allows cells to maintain their DNA content at the 2C level after each cell division. Here 1C is the DNA content of a haploid genome. However, certain cells undergoing differentiation increase their DNA contents to 4C or higher as a result of endoreduplication. It is thought to be a process in which chromosomal DNA is successively duplicated in the absence of mitosis. Plants exhibit endoreduplication more frequently than animals. Endoreduplication often occurs during the differentiation of cells that are highly specialized in their morphology or metabolism. An *Arabidopsis thaliana* trichome, a large branched cell on the surface of aerial organs (Figure 1), generally has a DNA content of 32C. Maize endosperm cells, which accumulate starch and storage proteins, usually undergo four to five successive endocycles during seed development. Other cells, such as those in leaves and roots, also exhibit high ploidy. *Arabidopsis* cotyledons and leaf pavement cells have ploidy levels from 2C to 32C and from 2C to 16C, respectively. Moreover, the ploidy levels of *Arabidopsis* hypocotyls vary depending on growth conditions, with levels of 2C to 8C under normal light conditions and 2C to 16C in darkness.

Although the involvement of various cell cycle-related proteins in endoreduplication has been shown, it is still unclear which proteins play key regulatory roles in endoreduplication, especially in the process of terminating endocycle succession at the appropriate ploidy levels. To identify key regulators of endoreduplication in plants, we searched for cell cycle-related genes expressed during *Arabidopsis* trichome development, in which endoreduplication occurs instead of the mitotic cell cycle. *CDKA;1* has been revealed to be expressed during trichome devel-

opment [1]. During the course of identifying cyclins that are involved in endoreduplication, we found that the promoter of a cyclin A gene, *CYCA2;3*, is active not only in proliferating tissues but also in developing trichomes in the termination period of endoreduplication. Null mutations of *CYCA2;3* semidominantly promoted endocycles and increased the ploidy levels achieved in mature organs, but they did not significantly affect the proportion of cells that underwent endoreduplication. Consistent with these characteristics, expression of the *CYCA2;3*-GFP fusion protein restrained endocycles in a dose-dependent manner. Moreover, a mutation in the destruction box of *CYCA2;3* stabilized the fusion protein in the nuclei and enhanced the restraint. These results indicate that *CYCA2;3* acts as a key regulator of ploidy levels in *Arabidopsis* endoreduplication, presumably through suppressing endocycle succession [2].

[1] Imajuku Y, Ohashi Y, Aoyama T, Goto K, and Oka A, *Plant Mol. Biol.* **46**, 205-213 (2001).

[2] Imai K, Ohashi Y, Tsuge T, Yoshizumi T, Matsui M, Oka A, and Aoyama T, *Plant Cell*, **18**, 382-396 (2006).

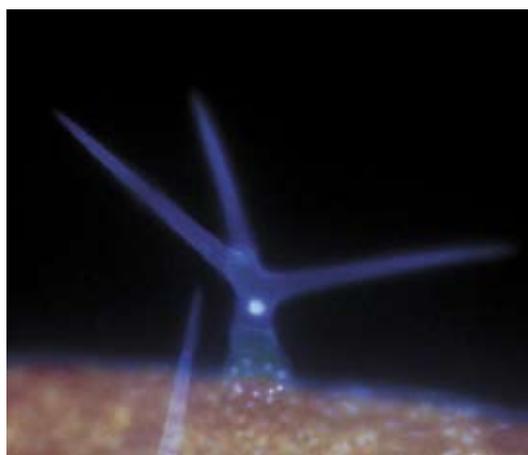


Figure 1. Microscopic observation of a trichome protruding from an *Arabidopsis* leaf surface. The pale blue circular body is the 32C nucleus visualized by DAPI staining.

Aoyama T, Information Transfer from Soil Environmental Signal towards Regulation of Root-hair Formation, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2008.

Aoyama T, Morphological and Functional Differentiation of Root Hairs for Nutrient Absorption, Exploratory Research Grant from Institute of Sustainability Science, 1 April 2006–31 March 2008.

Tsuge T, Novel Regulation Linking Plant Morphogenesis to Environmental Response, Kyoto University Start-up Fund, 1 January–31 March 2006.

Tsuge T, A Novel Mechanism of COP9 Signalosome Controlling Adaptive Responses, Grant-in-Aid for Scien-

tific Research (C), 1 April 2006–31 March 2008.

Tsuge T, Genetic Networks for Dorsal/Ventral and Width/Length Determination of the Leaf, Heiwa-Nakajima Foundation, 1 April 2006–31 March 2007.

Tsuge T, Stress-Response-Controlling Factor (COP9 Signalosome) Involved in Regulation of both Human Carcinogenesis and Plant Photomorphogenesis, The Naito Foundation, 1 December 2006–30 September 2008.

Award

Tsuge T, Awarded Guest Professor of Brain Korea 21 Silver-Bio Research Center, Dong-A University, Busan Korea, 1 March 2006–28 February 2007.

Division of Biochemistry - Chemical Biology -

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University of California, San Francisco of Cellular & Molecular Pharmacology, USA, 26 July 2006

Prof CHOO, Hea-Young
Prof MUIR, Thomas

Ewha Womans University College of Pharmacy, Korea, 12 October–12 December 2006
Rockefeller University of Biochemistry and Structural Biology, USA, 9 September 2006

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 2006)

Presentations

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, Aging and Cancer Genome Research Work Shop, Sendai, Japan, 20 January 2006.

Chemical Biology by Small Synthetic Compounds, Uesugi M, 7th Drug Discovery Vision Symposium, Tokyo, Japan, 23 February 2006.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, 86th Annual Meeting of the Chemical Society of Japan, 27 March 2006.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, 126th Annual Meeting of the Pharmaceutical Society of Japan, 29 March 2006.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, ICOB-5 & ISCNP-25 IUPAC, Kyoto, Japan, 27 July 2006.

Chemical Biology by Small Synthetic Compounds, Uesugi M, Genomic Drug Discovery Forum, Kyoto, Japan, 19 September 2006.

Chemical Biology by Small Synthetic Compounds, Uesugi M, JSPS Genome Technology Symposium, Tokyo, Japan, 26 September 2006.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, Senri Life Science Seminar, Osaka, Japan, 29 September 2006.

Chemical Biology by Small Synthetic Compounds, Uesugi M, 2nd Forum for Pharmaceutical Technology Innovation, Kyoto, Japan, 13–14 October 2006.

Chemical Biology of Gene Expression and Cell Differentiation, Uesugi M, 21st International Biohybrid Symposium, Yokohama, Japan, 1 November 2006.

Chemical Biology of Gene Expression, Uesugi M, 43th

Small-molecule-initiated Biology

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

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

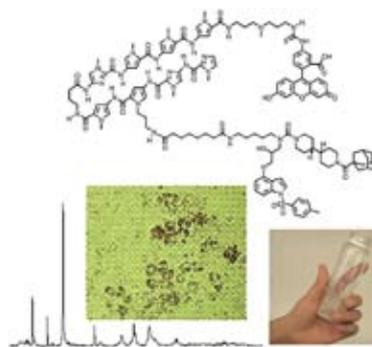
Discovery of synthetic small molecules that modulate transcription. Our group has discovered by screening chemical libraries a unique small-molecule modulator of transcription. The synthetic molecule we named “adamanolol” represents the first small molecules that modulate gene transcription by targeting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

Wrenchnolol mimics an alpha-helical activation domain of transcription factor ESX: it may serve as a small-molecule activation module when coupled with a DNA binding molecule. Our group, as a collaboration with Prof. Dervan in Caltech, has recently succeeded in designing a

completely organic, synthetic transcription factor that activates transcription. This work demonstrates that it is possible to generate a transcription factor out of organic compounds.

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

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



International JPS · PEM4, Yokohama, Japan, 6 November 2006.

Chemical Biology by Small Synthetic Compounds, Uesugi M, 3rd Combinatorial Bioengineering Conference, Osaka, Japan, 10 November 2006.

Grants

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

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

Uesugi M, Methods for Isolating Target Proteins of

Small Molecules, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2008.

Uesugi M, Intracellular Imaging of Small Molecules, Industrial Technology Research Grant Program by NEDO, 1 June 2006–20 March 2008.

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

Award

Uesugi M, Tokyo Techno-Forum 21Gold Medal Award, Small-molecule Based Chemical Genetic Research for Biological Investigation, 12 April 2006.

Division of Environmental Chemistry - Molecular Materials Chemistry -

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Visitors

Prof MACDONALD, Peter M University of Toronto, Canada, 13–18 October 2006

Prof BECKHAM, Haskell W Georgia Institute of Technology, USA, 24–29 November 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Noncrystalline Structure of Polymers Observed by High-Resolution Solid-State NMR, Horii F, Research Group of Fiber Materials, Soc. Polym Sci., Jpn., 1 March, (Invited).

Ordered and Disordered Structure of Native Cellulose Revealed by Solid-State NMR, Horii F, ACS Annual Meeting, 27 March, (Invited).

New Developments of the Characterization of Polymer Materials by High Magnetic-Field NMR, Horii F, 55th Symposium on Macromolecules, Soc. Polym Sci., Jpn., 21 September, (Invited).

From Simple to Advanced Solid-State NMR: the Analysis of Structure and Dynamics of Materials in Organic Devices, Kaji H, The 45th Annual Meeting of the NMR Society of Japan, 22 November (Invited).

Theoretical Study of Chemical Shift Changes by Cationization of TPD, a Hole Transport Material in Organic LEDs, Yamada T, Tsukamoto N, Kusaka Y, Kaji H, Horii F, 55th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 21 September.

Solid-State ^2H NMR Detection of *N,N'*-diphenyl-*N,N'*-di(*m*-tolyl)benzidine Thin Films, a Hole-Transport Material in Organic LEDs, Sesei T, Mino A, Kaji H, Horii F, 55th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 20 September.

Preparation and Structure of Nanocomposites Composed of Cellulose Microfibrils and Imogolite Nanotubes, Hirai A, Ikuno M, Horii F, Donkai N, Tsuji M, Polychar-14, 21 April.

Phase Behavior of Aqueous Suspensions of Tunicate Cellulose Nanofibers, Hirai A, Inui O, Ikuno M, Horii F,

Super-High Field Solid-State NMR Characterization of Hydrogen Bonding of Native Cellulose

We are developing new high-resolution solid-state ^1H NMR methods to characterize hydrogen bonding by using the world-highest 930 MHz solid-state NMR spectrometer in NIMS at Tsukuba. One method is ^1H homonuclear dipolar decoupling under relatively high magic angle spinning (MAS). Phase-modulated Lee-Goldburg (PM-LG) and eDUMB pulses were evaluated in detail but the resolution of the spectra thus obtained was found not to be very high compared to the ^1H combined rotation and multiple pulse spectroscopy (CRAMPS) spectra measured at 400 MHz. A new 2 mm MAS probe is now being developed to enhance the spectral resolution. Nevertheless, the ^{13}C - ^1H heteronuclear correlation (HETCOR) spectrum revealed that possible OH protons are well correlated with the corresponding C2, C3, and C6 carbons for tunicate cellulose as shown in Fig. 1 and the OH resonance lines in the ^1H CRAMPS spectrum are successfully assigned by using these correlations.

Another method is CP/MAS ^2H NMR spectroscopy newly developed by Mizuno et al. We successfully applied this method to the characterization of OH-deuterated tunicate and *Glaucozystis* celluloses which preferentially contain cellulose I_β and I_α crystals, respectively.

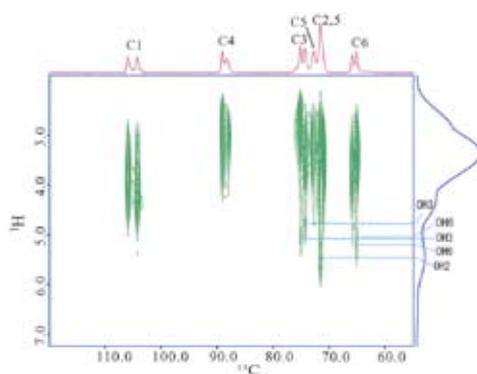


Figure 1. ^{13}C - ^1H HETCOR spectrum for tunicate cellulose.

Tsuji M, 55th Annual Meeting, Soc. Polym. Sci., Jpn., 24 May.

Formation and Structure of Liquid Crystal in Aqueous Suspensions of Sulfuric Acid Hydrolyzed Cellulose, Hirai A, Inui O, Ikuno M, Horii F, Tsuji M, 55th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 21 September.

Grants

Horii F, Precise Solid-State NMR Analyses of Noncrystalline Organized Structure and Dynamics of Polymer Functional Materials, Grant-in-Aid for Scientific Research

Formation and Structure of Liquid Crystal in Aqueous Suspensions of Tunicate Cellulose Nanofibers

Effective utilization of cellulose is a subject of great importance. Tunicate cellulose nanofibers prepared by sulfuric acid hydrolysis of purified mantles of tunicin are rodlike in appearance, 1-3 μm long and 15-30 nm wide. Aqueous suspensions of nanofibers separate into an isotropic and liquid crystalline phases above the concentration of 0.3 wt%. In particular, suspensions ranging in a cellulose concentration from 1 to 3 wt% are separated into three layers (Figure 2). The upper layer is the isotropic phase. The bottom layer exhibits a fingerprint-like pattern characteristic of the chiral nematic phase. Upon application of the horizontal field of 10T for 48h, the fingerprint texture in the bottom layer aligns with its helical axis being parallel to the applied magnetic field. The middle layer is also an anisotropic phase, but a fingerprint pattern is not observed. The distributions of the size of the nanofibers investigated by TEM are not different between the middle and bottom layers. However, a significant difference in ζ -potential is observed between them. Hence, it is concluded that surface charge density is the main factor to exhibit the different textures between the middle and bottom layers.

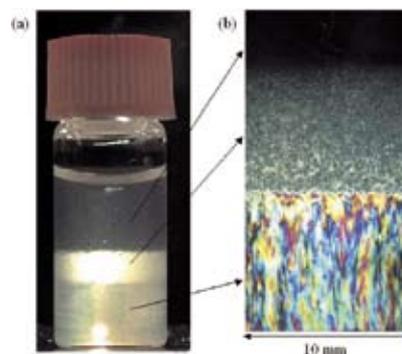


Figure 2. (a) Aqueous suspension of tunicate cellulose microfibrils with a concentration of 2.0 wt%. Three layers are formed. (b) Crossed-polar images of three layers of panel a.

(B) (2), 1 April 2004–31 April 2006.

Horii F, Hybridization Utilizing Hierarchical Structure of Microbial Cellulose by a Newly Developed Microbiological System, Grant-in-Aid for Scientific Research, 1 April 2004–31 April 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 -

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NAKATSUKA, Seiji (D2)

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Prof LI, Yuan-Hui University of Hawaii, USA, 1–3 April 2006

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. The study also covers hydrothermal activity and deep biosphere. Major parts of these studies are based on field works. (ii) Iron uptake mechanism of phytoplankton. (iii) Ion recognition. (iv) Simulation of chemical reactions.

Research Activities (Year 2006)

Presentations

Geochemistry of Bioactive Trace Metals during the Mesoscale Iron Enrichment in the Subarctic Western North Pacific Gyre (SEEDS I and II), Nakatsuka S, Kinugasa M, Sohrin Y, Nishioka J, Takeda S, Tsuda A, 2006 Ocean Sciences Meeting, 20 February 2006.

Spatial and Temporal Distribution of Fe, Ni, Cu and Pb along 140E in the Southern Ocean in 2001/2002 Austral Summer, Sohrin Y, Lai X, Norisuye K, Mikata M, Minami T, Bowie A R, 2006 Ocean Sciences Meeting, 20 February 2006.

Novel Determination of Pd, Pt and Au in the Western North Pacific Seawater, Sohrin Y, Sato T, Norisuye K, Hatta M, Zhang J, 2006 Western Pacific Geophysics Meeting, 27 July 2006.

Inter-Basin Fractionation on the Distributions of Bioactive Trace Metals and Metal/Nutrient Ratios in the Sulu Sea, South China Sea and Western North Pacific, Norisuye K, Ezoe M, Nakatsuka S, Sohrin Y, 2006 West-

ern Pacific Geophysics Meeting, 27 July 2006.

Determination and Distribution of Zr, Hf, Ta and W in the North Pacific Ocean, Firdaus M L, Norisuye K, Sato T, Urushihara S, Nakagawa Y, Sohrin Y, 16th Annual V.M. Goldschmidt Conference 2006, 30 August 2006.

Determination of Trace Metals in Seawater Using ICP-MS after Concentration with NOBIAS Chelating Absorbent Column, Minami T, Urushihara S, Sohrin Y, The 55th Annual Meeting of the Japan Society for Analytical Chemistry, 22 September 2006.

Molecularly Imprinted Sol-Gel Absorbent for the Separation of Divalent Metal Ions, Umetani S, Taguchi Y, Kurahashi K, The 55th Annual Meeting of the Japan Society for Analytical Chemistry, 22 September 2006.

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.

Distribution of Zr, Hf, Nb, Ta, Mo and W in the North Pacific Ocean

Comprehensive information of trace elements in seawater is important for understanding the marine system. Zr, Hf, Nb, Ta, Mo and W are adjacent elements in the periodic table. In seawater, Zr, Hf, Nb and Ta are dominated by hydroxide species such as $Zr(OH)_5^-$, $Hf(OH)_5^-$, $Nb(OH)_6^-$ and $Ta(OH)_6^-$, while Mo and W are present as MoO_4^{2-} and WO_4^{2-} . The hydroxide dominated elements are more reactive than the oxyacid dominated elements and thought to have potential as oceanographic tracers of external sources, physical mixing, and scavenging removal processes.

We have developed a solid-phase extraction method using TSK-8HQ as chelating resin to concentrate these elements in seawater [1]. The greatest advantage of this resin is its endurance to 5 M HF, since this is an effective eluent for the six metals. The analytes were quantitatively concentrated from 250 mL seawater with a 50 fold concentration factor through the column extraction and evaporation. Seawater samples were collected from the western North Pacific during the MR05-01 cruise of R/V Mirai (Figure 1) using a CTD carousel, on which Niskin-X samplers were mounted. The interior of the samplers was coated with Teflon and cleaned with detergent and HCl. A portion of seawater for dissolve species (D) was filtered through a 0.2 μm Nuclepore filter and acidified to pH 2.2 with HCl and HF. A portion of seawater for acid-dissolvable species (AD) was acidified without filtration. The acid-dissolvable element includes dissolved species and a labile particulate fraction dissolved during storage. It would contain species, such as iron hydroxides, adsorbed on clay minerals and incorporated in organism.



Figure 1. MIRAI; the research vessel used for the collection of sample.

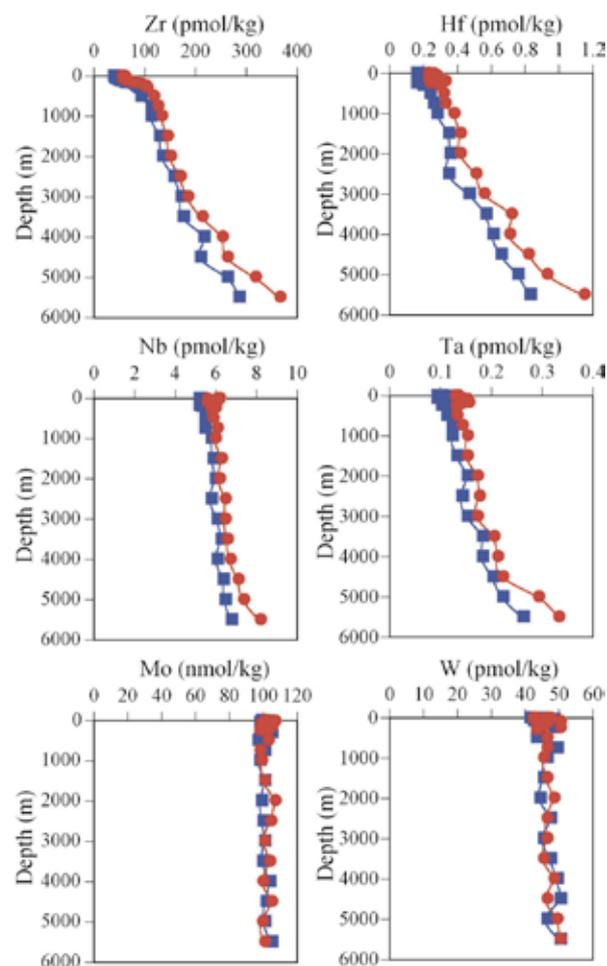


Figure 2. Vertical profiles of dissolved (■) and acid-dissolvable (●) elements at station K-4.

At station K-4 (35°N, 160°E), Zr and Hf show systematic enrichment with depth, Nb shows slight depletion in surface water, Ta shows enrichment in bottom water, whereas Mo and W show conservative vertical profiles (Figure 2). AD to D ratio for Zr, Hf, Nb and Ta are higher in the surface and bottom water compared to mid-depth, whereas concentrations for Mo and W show no significant difference between D and AD. We also determined the concentrations in coastal seawater, rain, river and hot spring water and observed that dissolved Zr/Hf, Nb/Ta and Mo/W ratios increase in the order of crust < river water < rain water < seawater. Thus, the mobility of Hf, Ta and W was lower than that of Zr, Nb and Mo.

[1] M. Lutfi Firdaus, K. Norisuye, T. Sato, S. Urushihara, Y. Nakagawa, S. Umetani and Y. Sohrin (2007) *Anal. Chim. Acta*, in press.

Norisuye K, Development of Analytical Method for Unstable Fe(II) in Seawater Based on *In situ* Preconcentration,

Grant-in-Aid for Young Scientists B, 1 April 2006–31 March 2007.

Division of Environmental Chemistry - Solution and Interface Chemistry -

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Prof KLEIN, Michael L

Prof GANGULY, Tapan

Institute for Molecular Science, Japan, 25–26 January 2006

University of Pennsylvania, USA, 16 June 2006

Indian Association for the Cultivation of Science, India, 23 August 2006

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 2006)

Presentations

In-situ NMR Spectroscopic Studies on Human Jurkat Cells, Nakahara M, Okamura E, Ninomiya K, Futaki S, Wakai C, Matubayasi N, Sugiura Y, 9th Eurasia Conference on Chemical Science, Antalya, Turk, 9–13 September.

Self-Diffusion of Supercritical Water in Extremely Low-Density Region, Nakahara M, the International Association for the Properties of Water and Steam, Witney, England, 3–8 September.

Free Energy of Solvation in the Method of Energy Representation, Matubayasi N, 16th Symposium on Thermophysical Properties, Boulder, USA, 30 July– 4 August.

Solvation Free Energy in Supercritical Water and Its Role toward Noncatalytic Reaction Control, Matubayasi N, 4th International Symposium of Molecular Thermodynamics and Molecular Simulation, Makuohri, Japan, 22–25 May.

Grants

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

Nakahara M, Development of Technology for Hydrogen Production, Storage, and Transportation of Hydrogen Using Hydrothermal Reactions of Formic Acid, ENEOS Hydrogen Trust Fund, 1 October 2006–30 September 2007.

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

Kinetic and Equilibrium Study on the Formic Acid Decomposition in Relation to the Water-Gas-Shift Reaction

Kinetics and equilibrium are studied on the hydrothermal decarbonylation and decarboxylation of formic acid, the intermediate of the water-gas-shift (WGS) reaction, in hot water at temperatures of 170–330 °C, in order to understand and control the hydrothermal WGS reaction (Figure 1). ^1H and ^{13}C NMR spectroscopy is applied to analyze as a function of time the quenched reaction mixtures both in the liquid and gas phases. Only the decarbonylation is catalyzed by HCl, and the reaction is first order with respect to both $[\text{H}^+]$ and $[\text{HCOOH}]$. Consequently, the reaction without HCl is first and a half (1.5th) order due to the unsuppressed ionization of formic acid. The HCl-accelerated decarbonylation path can thus be separated in time from the decarboxylation. The rate and equilibrium constants for the decarbonylation are determined separately by using the Henry constant (gas solubility data) for carbon monoxide in hot water. The rate constant for the decarbonylation is 1.5×10^{-5} , 2.0×10^{-4} , 3.7×10^{-3} , and $6.3 \times 10^{-2} \text{ mol}^{-1} \text{ kg s}^{-1}$, respectively, at 170, 200, 240, and 280 °C on the liquid branch of the saturation curve. The Arrhenius plot of the decarbonylation is linear and gives the activation energy as $146 \pm 3 \text{ kJ mol}^{-1}$. The equilibrium constant $K_{\text{CO}} = [\text{CO}] / [\text{HCOOH}]$ is 0.15, 0.33, 0.80, and 4.2, respectively, at 170, 200, 240, and 280 °C. The van't Hoff plot results in the enthalpy change of $\Delta H = 58 \pm 6 \text{ kJ mol}^{-1}$. The decarboxylation rate is also measured at 200–330 °C both in acidic and basic conditions. The rate is weakly dependent on the solution pH and is of the order of $10^{-4} \text{ mol kg}^{-1} \text{ s}^{-1}$ at 330 °C. Furthermore, the equilibrium constant $K_{\text{CO}_2} = [\text{CO}_2][\text{H}_2] / [\text{HCOOH}]$ is estimated to be $1.0 \times 10^2 \text{ mol kg}^{-1}$ at 330 °C.



Figure 1. Reaction scheme of water-gas-shift reaction.

Slowdown of H/D Exchange Reaction Rate and Water Dynamics in Ionic Liquid: Deactivation of Solitary Water Solvated by Small Anions in 1-Butyl-3-Methyl-Imidazolium Chloride

The H/D exchange reaction (Figure 2) and the rotational dynamics of heavy water (D_2O) are studied at 50 °C in the room-temperature ionic liquid, 1-butyl-3-methylimidazolium chloride ($[\text{bmim}][\text{Cl}]$), in the D_2O range of 3–55 M. The initial H/D exchange rates are observed as 1×10^{-7} , 4.5×10^{-6} , 1.0×10^{-5} , 4.1×10^{-5} , 1.1×10^{-4} and $3.7 \times 10^{-4} \text{ s}^{-1}$, respectively, at $[\text{D}_2\text{O}]$ of 2.8, 7.1, 8.1, 10.8, 15, and 25 M. The rate is very slow and less than 10^{-5} s^{-1} at $[\text{D}_2\text{O}]$ below $\sim 7 \text{ M}$. It steeply increases to the order of 10^{-4} s^{-1} for $7 \text{ M} < [\text{D}_2\text{O}] < 10 \text{ M}$, and linearly increases with $[\text{D}_2\text{O}]$ in the more water-rich region. The intercept of the linear region at $[\text{D}_2\text{O}] = \sim 9 \text{ M}$ is interpreted by considering that each chloride anion deactivates 1.6 equivalent water molecules due to the strong solvation (Figure 3). Correspondingly, the rotational correlation time of D_2O at $[\text{D}_2\text{O}] < 7 \text{ M}$ is one order of magnitude larger than that in water-rich conditions.

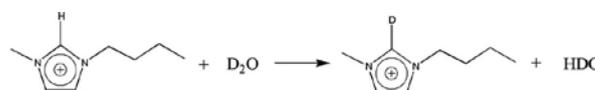


Figure 2. H/D exchange reaction scheme of $[\text{bmim}]$ cation.

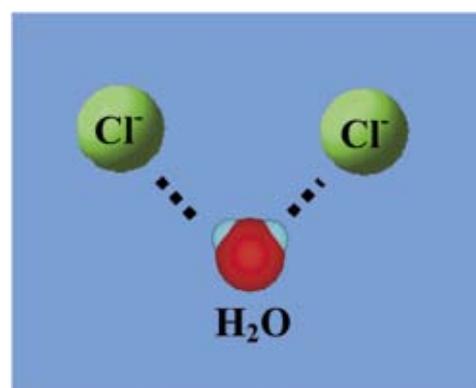


Figure 3. Schematic draw of the solvation of water by chloride anions.

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.

Wakai C, NMR Study on Dynamics of Water Molecule, Organic Molecules, and Ions in Ionic Liquids, Grant-in-

Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2008.

Award

Matubayasi N, Young Scientist Award, The Minister of Education, Culture, Sports, Science and Technology of Japan, 11 April.

Division of Environmental Chemistry - Molecular Microbial Science -

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



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Prof LIU, Hung-wen University of Texas at Austin, USA, 2 June–25 July 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Psychrotrophic Bacteria: Cold-Adaptation Mechanism and Applications, Esaki N, Kurihara T, Kawamoto J, Miyake R, Kitagawa M (Takara Bio Inc.), Kato I (Takara Bio Inc.), International Conference on Alpine and Polar Microbiology, 27 March.

A Comparative Study between Selenocysteine Lyase and Cysteine Desulfurase, Mihara H, Kurokawa S, Omi R, Kurihara T, Miyahara I (Osaka City Univ.), Hirotsu K (Osaka City Univ.), Esaki N, 8th International Sympo. Selenium in Biology and Medicine, 26 July.

Cold-adaptation Mechanism of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, and Its Applications, Kurihara T, Kawamoto J, Miyake R, Nagayasu M, Tani Y, Inomoto Y, Yamamoto K, Kitagawa M (Takara

Bio Inc.), Kato I (Takara Bio Inc.), Esaki N, Extremophiles 2006, 20 September.

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), 1 April 2005–31 March 2007.

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

Kurihara T, Conversion of Organofluorine Compounds with Microbial Enzymes: Mechanistic Analysis of the Enzyme Reactions and Their Application to Production of

The Cellular Function of Selenocysteine Lyase in Selenoprotein Synthesis

Enzymatic discrimination between selenium compounds and the corresponding sulfur compounds is important for cells to metabolize selenium compounds without interference by sulfur metabolism. Mammalian selenocysteine lyase (SCL) is a pyridoxal 5'-phosphate (PLP)-dependent enzyme that specifically acts on L-selenocysteine to yield L-alanine and selenium. The physiological relevance of the selenium-specific action of the enzyme, however, has remained unclear. To address the role of SCL in mammalian cells, we have used RNA-interference (RNAi) to deplete SCL and thereby assess its function in cell lines. We found that decreasing the level of SCL in HeLa cells results in significant reduction in protein levels of cytosolic glutathione peroxidase (cGPx) and activities of cGPx and thioredoxin reductase (TrxR). We also found that RNAi-mediated reduction of SCL induces cell growth inhibition even in the presence of selenomethionine, selenocysteine, selenite, or FBS in a serum-free medium. This result provides new insights into possible pathways for selenite metabolism. Overexpression of mouse SCL in HeLa cells elevated the activity of cGPx, suggesting that SCL is a rate-limiting enzyme in the synthesis of selenoproteins. These results demonstrate for the first time an essential role of SCL in selenoprotein biosynthesis in mammalian cells.

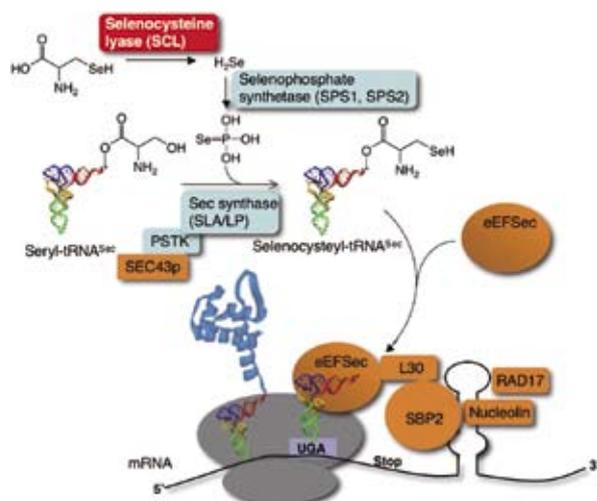


Figure 1. A proposed function of SCL in selenoprotein biosynthesis.

Construction of a Protein Expression System Operating at Low Temperatures by Using a Cold-Adapted Bacterium as the Host

Recombinant protein expression system working at low temperatures is expected to be useful for the production of thermolabile proteins as well as toxic enzymes whose activity can be suppressed by decreasing the temperature. We constructed a low-temperature expression system by using an Antarctic cold-adapted bacterium, *Shewanella livingstonensis* Ac10, as the host. We identified proteins abundantly produced at 4°C in this bacterium by two-dimensional gel electrophoresis and evaluated the promoters for these proteins to express foreign proteins. We used 27 promoters and a broad-host-range vector, pJRD215, to produce β-lactamase in *S. livingstonensis* Ac10. Maximum yield was obtained when the promoter for putative alkyl hydroperoxide reductase, AhpC, was employed and the recombinant cells were grown to the late stationary phase. The yield was 91 mg/L-culture at 4°C and 139 mg/L-culture at 18°C. We used this system to produce putative peptidases, PepF, LAP, and PepQ, and a putative glucosidase, BglA, from a psychrophilic bacterium, *Desulfotalea psychrophila* DSM12343. We obtained 48, 7.1, 28, and 5.4 mg/L-culture of these proteins, respectively, in a soluble fraction. The amount of PepF and PepQ produced by this system was higher than that produced by the *Escherichia coli* T7 promoter system, which is regarded as one of the most powerful protein expression systems currently available. This system would greatly contribute to fundamental and application studies of a number of proteins that can not be overproduced by conventional protein expression systems.

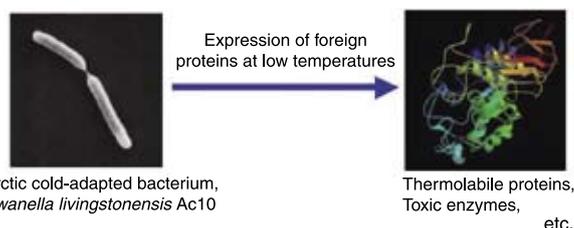


Figure 2. Protein expression at low temperatures by using an Antarctic bacterium, *S. livingstonensis* Ac10 as the host.

Useful Compounds and Bioremediation of Environments, Grant-in-Aid for Scientific Research (B), 1 April 2005–31 March 2008.

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

Division of Multidisciplinary Chemistry - Polymer Materials Science -

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



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Imperial College, UK, 27 March 2006
Albert-Ludwigs-Universität Freiburg, Germany, 24 April 2006
Instituto de Estructura de la Materia, CSIC, Spain, 30 June 2006
King's College, UK, 18 July 2006
SungKyunKwan University, Korea, 18 August 2006

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 2006)

Presentations

Phase Separation and Dewetting in Polymer Blend Thin Films, Ogawa H, Kanaya T, Nishida K, Matsuba G, 3rd International Workshop on Dynamics in Confinement, Grenoble, France, 23–26 March.

Crystallization Process of Isotactic Polypropylene under Shear Flow, Ogino Y, Matsuba G, Nishida K, Kanaya T, 55th Annual Meeting of the Society of Polymer Science, Japan, Nagoya, 20–22 May.

Phase Separation and Aggregation in Polyelectrolyte Solutions (Invited), Nishida K, Tsubouchi T, Kanaya T, 11th International Symposium on Colloidal and Molecular Electro-Optics, Kyoto, 25 May.

Crystal Structure and the Melting Behavior of Poly(L-lactic acid), Kawai T, SAS2006, Kyoto, Japan, 9–13 July.

Structural Formation Process of Poly(ethylene tere-

phthalate) under Shear Flow Using Time-Resolved Depolarized Light Scattering Technique, Takahashi N, Matsuba G, Nishida K, Kanaya T, 52nd Meeting of Polymer Science, Kobe, 21 July.

Structure Analysis of Organic-Inorganic Hybrid Low-Melting Glasses as Studied by Static and Dynamic Light Scattering, Iseki T, Inoue R, Matsuba G, Nishida K, Kanaya T, Kakiuchida H, Takahashi M, 55th Discussion Meeting, the Society of Polymer Science Japan, Toyama, 20–22 September.

Precise Analysis for Fiber Structure with Scattering Methods, Matsuba G, Ogino Y, Nishida K, Kanaya T, The Sino-Japanese Fiber Symposium, Xiamen, P. R. China, 23–25 October.

Dynamical Properties of Polystyrene Thin Films, Inoue R, Kanaya T, Nishida K, Tsukushi I, Jülich Soft Matter

Crystallization of Polyethylene Blends of Ultra-high and Low Molecular Weight Components under Shear Flow

Time resolved small-angle X-ray scattering (SAXS) measurements were performed on crystallization processes of ultra-high and low molecular weight polyethylene blends after applying pulse shear in order to clarify effects of ultra-high molecular component on shish-kebab structure formation. Anisotropic scattering pattern due to kebab-structure formation is observed above a certain critical concentration of ultra-high molecular weight polyethylene (Figure 1). The critical concentration is about ~ 0.1 wt% independent of the crystallization temperature below 125°C , while it increases with the crystallization temperature above 125°C . Analyzing the results it is revealed that the shish-kebab formation is dominated by entanglements of the ultra-high molecular weight chains as well as competition between the crystallization rate and the relaxation rate of entanglements.

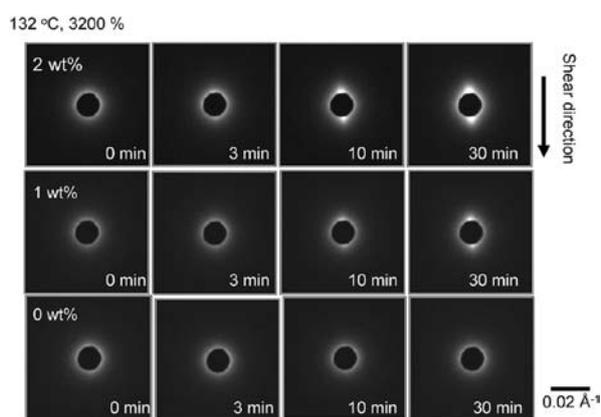


Figure 1. Time evolution of 2D SAXS profiles in various ultra-high molecular weight polyethylene concentrations.

Phase Separation and Dewetting in Polymer Blend Thin Films

We have studied morphology and kinetics of phase separation as well as dewetting in polystyrene (PS) and poly(vinyl methyl ether) (PVME) blend thin films, which

are very different from those of bulk blends, using time-resolved light scattering (LS), optical microscope (OM) and atomic force microscope (AFM). Time evolution of LS intensity is well described by kinetics of spinodal decomposition type phase separation in the films above $\sim 1 \mu\text{m}$ (Figure 2(a), (d)) while confinement effects were recognized below about $10 \mu\text{m}$. As the film thickness decreases below $\sim 1 \mu\text{m}$, a peak in LS profile characteristic to phase separation once disappears (Figure 2(b)). In this thickness region, phase separation and dewetting must competitively occur, resulting in the irregular pattern (Figure 2(e)). As the thickness further decreases below about $\sim 100 \text{ nm}$, a scattering peak is again observed (Figure 2(c)), meaning the dewetting occurs preferentially (Figure 2(f)), which was confirmed by AFM measurements.

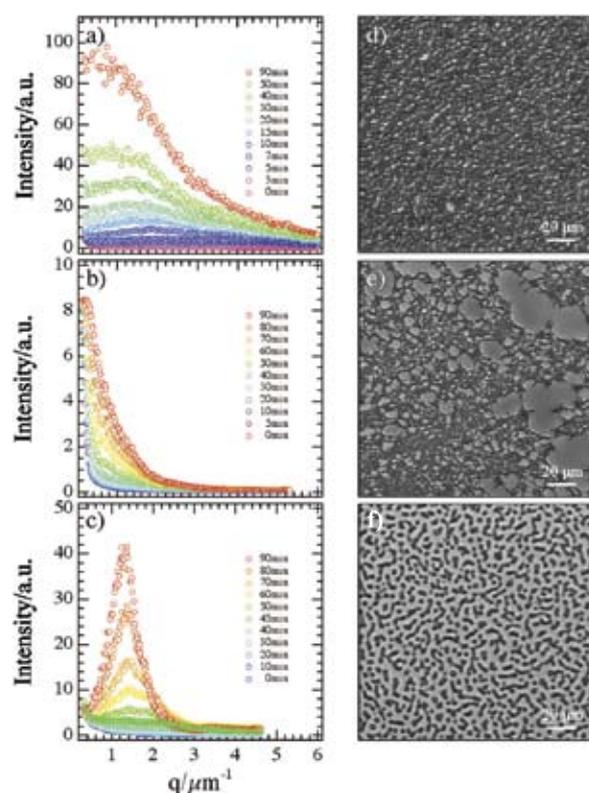


Figure 2. Time-resolved LS profiles for PS/PVME blend films with the thickness of $66 \mu\text{m}$ (a), 470 nm (b) and 40 nm (c) (left) and OM images $66 \mu\text{m}$ (d), 470 nm (e) and 40 nm (f) after 90 minutes in two phase region (right).

Days 2006, Bonn, Germany, 14–17 November.

Grants

Kanaya T, Collaboratory on Electron Correlation toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2004–31 March 2006.

Kanaya T, Higher Order Structure Formation in Induc-

tion Period of PLA Crystallization and in External Fields, Collaboration Research with Toyota Motor Corporation and Toyota CRDL., INC, 15 January 2003–31 March 2008.

Matsuba G, Observation of Shish-kebab Structural Formation Processes of Polymers with Neutron Scattering Technique, Grant-in-Aid for Young Scientists (B), 1 April 2005–31 March 2007.

Division of Multidisciplinary Chemistry - Molecular Rheology -

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DEMÉ, Bruno Institut Laue-Langevin, Grenoble, France, July 2006
SUN, Kang Shanghai Jiao Ton University, China, P.R., 24–28 July 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Non-Newtonian Behavior of Diblock and Triblock Copolymer Solutions, Watanabe H, APS Annual Meeting, Baltimore, MD, USA, March 2006.

Constraint Release in Star/Star Blends and Partial-DTD in Monodisperse Star Systems, Watanabe H, AERC06, Hersonisos, Crete, Greece, April 2006.

Dynamics of Monofunctional Polybutadienyl Lithium Chains Aggregated in Benzene, Watanabe H, AERC06, Hersonisos, Crete, Greece, April 2006.

Non-Newtonian Behavior of Diblock and Triblock Copolymer Solutions, Matsumiya Y, AERC06, Hersonisos, Crete, Greece, April 2006.

Dielectric Studies for Predicting Viscoelastic Properties of Polymers under Supercritical CO₂, Inoue T, Macro 2006, Rio de Janeiro, Brazil, July 2006.

Non-Newtonian Behavior of Diblock and Triblock

Copolymers, Watanabe H, PPS 22, Yamagata, July 2006.

Molecular Picture of Dynamic Tube Dilation for Entangled Polymers –Coarse-Graining of Length Scale Consistent with Time Scale–, Watanabe H, Yukawa Institute for Theoretical Physics (YITP) Workshop, Kyoto, July 2006.

Transient Conformational Change of Bead-spring Ring Chain during Creep Process, Watanabe H, SOR Meeting, Portland, MA, USA, October 2006.

Constraint Release in Star/Star Blends and Partial-DTD in Monodisperse Star Systems, Watanabe H, SOR Meeting, Portland, MA, USA, October 2006.

Grants

Watanabe H, Creation of Non-equilibrium Soft Matter Physics: Structure and Dynamics of Mesoscopic Systems, Grant-in-Aid for Scientific Research on Priority Areas,

Constraint Release in Moderately Entangled Monodisperse Star Polyisoprene Systems

For examination of a constraint release (CR) contribution to relaxation in monodisperse systems of moderately entangled 6-arm star polyisoprenes (PI), viscoelastic measurements were conducted for blends of these star PI and a high molecular weight (M) linear PI. In the blends, the linear PI was dilute and entangled only with the matrix star chains. The terminal relaxation of this dilute linear probe occurred through competition of reptation and Rouse-type CR, as confirmed from its relaxation mode distribution. The probe relaxation time τ_{probe} measured in the blends was utilized in the following way to elucidate the CR relaxation of the star matrices. Since the CR time τ^{CR} of the star matrix is expressed as $(2N_a)^2\tau_{\text{lifc}}$ with $2N_a$ and τ_{lifc} being the entanglement number per two arms (span length) and the effective entanglement lifetime in the system, τ^{CR} can be evaluated if the τ_{lifc} value is known. For determination of the τ_{lifc} value, the τ_{probe} data of the linear probe in the star matrices was compared with the τ_{probe} data of the *same* probe in linear PI matrices (Figure 1) under a molecular idea that τ_{lifc} should be the same in a *pair* of star and linear matrices giving the same τ_{probe} value. The molecular weight $M_{\text{L,mat}}$ of the linear matrix paired with each star matrix was thus specified as indicated with the filled squares in Figure 1, and the value of τ_{lifc} in the star matrix was determined by utilizing this $M_{\text{L,mat}}$ value in an empirical equation of τ_{lifc} in the linear matrices ($\tau_{\text{lifc}} = 2.5 \times 10^{-18} M_{\text{L,mat}}^3$ s at 40°C). For the monodisperse systems of the star PI, the $\tau^{\text{CR}} (= (2N_a)^2\tau_{\text{lifc}})$ thus evaluated was close to the measured relaxation time (Figure 2), indicating that the CR mechanism significantly contributes to the star relaxation. This result was in harmony with the validity of the molecular picture of partial dynamic-tubedilation (p-DTD) confirmed for the star PI.

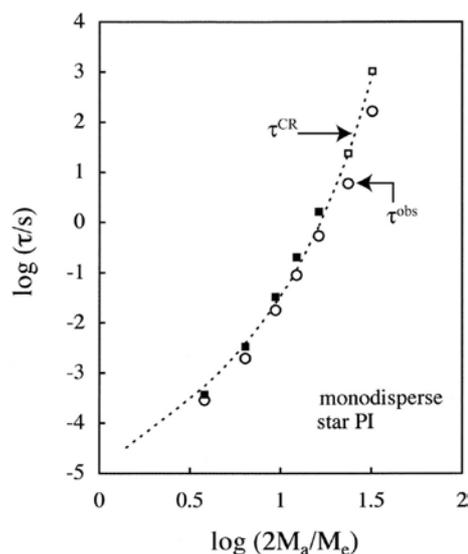


Figure 1. Plots of the terminal viscoelastic relaxation time τ_{probe} of the dilute linear probe in 6-arm star PI matrices (large unfilled squares) and/or linear PI matrices (circles) at 40°C. The symbols with pip indicate that the probe exhibited pure CR behavior in the given matrices.

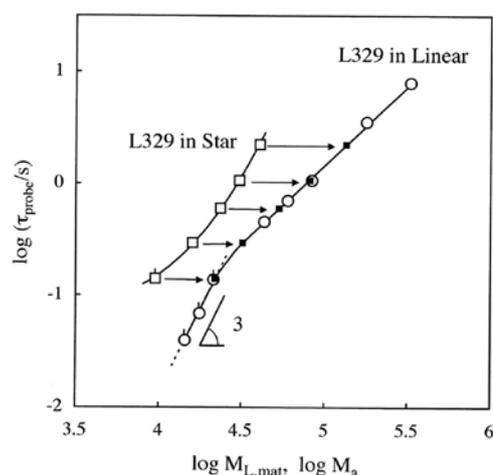


Figure 2. Comparison the viscoelastic CR relaxation time τ^{CR} for monodisperse systems of star and linear PI chains with the observed terminal relaxation time τ^{obs} (circles) at 40°C.

October 2006–March 2011.

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.

Division of Multidisciplinary Chemistry - Molecular Aggregation Analysis -

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MORIE, Jun (M2)
SASAMURA, Tatsuya (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 spectroscopies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous structures in microcapsules, biopolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2006)

Presentations

Dielectric Properties of Biological Cells and Tissues: Monitoring and Modeling, Asami K, International Conference of Biosensing and Biodynamics: From Basics to Applications (Bucharest, Romania), 18–21 May.

Observation of Electronic Structure of Frontier States in Organic Semiconductor Thin Films, Sato N, Yoshida H, Murdey R J, Workshop on Charge Carrier Injection and Transport Phenomena in Organic Thin Films and the 10th European Conference on Organised Films (ECOF-10) (Riga, Latvia), 20–24 August.

Dielectric Properties of Osmotically-lysed Erythrocytes, Asami K, 4th Conference of International Dielectric Society & 9th Conference of Dielectric and Related Phenomena (Poznan, Poland), 3–7 September.

Structure and Electronic Structure of Unoccupied States in Pentacene Thin Films, Sato N, Yoshida H, Murdey R J, The 13th International Conference on Solid Films and Surfaces (ICSFS-13) (San Carlos de Bariloche, Argentina), 6–10 November.

Structure of Pentacene Thin-Film Phase Determined with X-ray Diffraction Reciprocal Space Mapping Method (in Japanese), Yoshida H, Inaba K (Rigaku Co.), Sato N, The 15th Organic Crystals Symposium (Matsuyama, Japan), 24–25 November.

IPES and UPS Studies on Frontier Electronic States in Organic Semiconductor Thin Films, Sato N, Yoshida H, Murdey R J, Asian Pacific Conference on Surface Science & Engineering (Hong Kong, China), 19–21 December.

Grants

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

Asami K, Dielectric Spectroscopy of Blood Cells, Collaboration Research with Sony Corporation (Life Science Laboratory, Material Laboratories), 10 November 2006–31 March 2007.

Polymorphic Phase Transition of the Crystal of a Highly Amphoteric Polar Molecule

{4-[4,5-Bis-(methylsulfanyl)-1,3-dithiol-2-ylidene]-cyclohexa-2,5-dien-1-ylidene}malononitrile (BMDCM) grouped into highly amphoteric polar molecules was found to show polymorphism: Solution- and vapor-grown crystals are blue plate-formed and green needle-formed ones, respectively. X-ray structural analyses revealed that the space groups of the former and the latter crystals are triclinic $P\bar{1}$ and monoclinic $P2_1/n$, respectively. BMDCM molecules are stacked along a -axis in the head-to-tail manner to form π electron columns in both crystals. The orientation relation among the stacked molecular columns is different between the two crystals; all the molecular long axes are parallel to each other in the solution-grown crystal, however, the molecular long axes of a column are almost normal to those of the nearest column in the vapor-grown one. Further, the solution-grown crystal exhibited color change from blue to green when heated at 493 K. Then we examined powder X-ray diffraction patterns of the crystal before and after the heat treatment and confirmed that the pattern obtained for the heated crystal was almost the same as that for the vapor-grown crystal. Thus we have found the polymorphic phase transition of BMDCM crystal induced thermally. It is notable that a larger solution-grown crystal showed the phase transition with keeping the crystalline appearance in spite of the large difference in the packing manner of molecular stacking columns between the two polymorphs. Such a difference and the phase transition behavior attract our attention in terms of electronic properties and molecular dynamics in the solid state so that further studies on these problems are in progress.

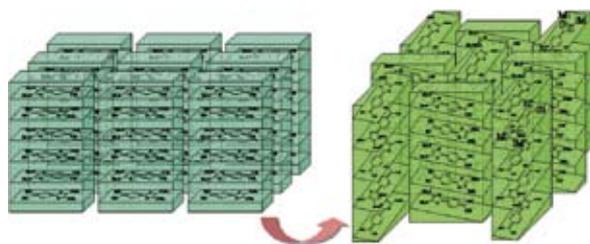


Figure 1. Schematic of the change in packing manner of molecular stacking columns via polymorphic phase transition of BMDCM crystal.

Ion Channels of N-Terminally-Linked Alamethicin Dimers: Enhancement of Cation-Selectivity by Substitution of Glu for Gln at Position 7

Alamethicin forms voltage-gated ion channels that have moderate cation-selectivity. The enhancement of the cation-selectivity by introducing negatively charged residues at positions 7 and 18 has been studied using the tethered homodimers of alamethicin with Q7 and E18 (di-alm-Q7E18) and its analog with E7 and Q18 (di-alm-E7Q18) (Figure 2). In the dimeric peptides, monomer peptides are linked at the N-termini by a disulfide bond. Both the peptides formed long lasting ion channels at *cis*-positive voltages when added to the *cis*-side membrane. Their long open duration enabled us to obtain current-voltage ($I-V_m$) relations and reversal potentials at the single-channel level by applying a voltage ramp during the channel opening. The reversal potentials measured in asymmetric KCl solutions indicated that ionized E7 provided strong cation-selectivity whereas ionized E18 little influenced the charge selectivity. This was also the case for the macroscopic charge selectivity determined from the reversal potentials obtained by the macroscopic $I-V_m$ measurements. The results are accounted for by stronger electrostatic interactions between permeant ions and negatively-charged residues at the narrowest part of the pore than at the pore mouth.

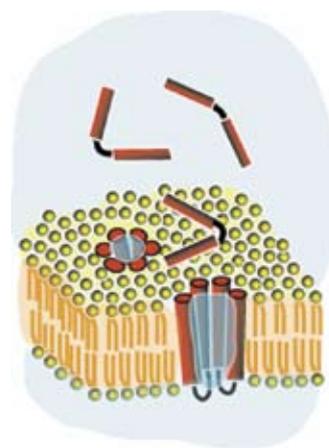


Figure 2. Ion channels formed by covalently-linked alamethicin dimers in a lipid bilayer.

Yoshida H, Controlling Reactivity and Diffusion at 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 -

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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 2006)

Presentations

Regulation of Membrane Phospholipid Dynamics and Its Role in Cell Size Control. Kato U. The 9th Membrane Research Forum. 15–17 March, Kyoto.

Dynamics of Membrane Phospholipids and Its Role in Cytoskeletal Reorganization. Inadome H., Kubo A., Kato U., Umeda M. 28th Symposium on Biomembrane-Drug Interaction. 9–10 November, Shizuoka.

Role of Phospholipid Flip-flop in Cell Polarization. Umeda M. The 46th Annual Meeting of the American Society for Cell Biology. 9–13 December, San Diego, USA.

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

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

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.

Regulation of Membrane Phospholipid Dynamics and Its Role in Control of Cell Motility

The basic structure of biological membranes is the lipid bilayer in which phospholipids distribute asymmetrically between the two leaflets of the bilayer. Although this asymmetry is regulated by the transbilayer movement of phospholipids occurred by a protein-mediated process, its physiological significance and molecular mechanisms are largely unknown. To identify the molecules that regulate the movements of membrane phospholipids, we established a series of yeast mutants with disordered organization of membrane phospholipids. By analyzing these mutants, we have identified a novel membrane protein, designated Ros3p, which is required for the transbilayer movement of phospholipids across the yeast plasma membrane. Ros3p is highly conserved in various organisms, implying a general role for cellular functions. To investigate its biological functions, we have cloned mROS3, a mammalian homolog of Ros3p. Overproduction of mROS3 facilitated the membrane ruffling and cell motility in CHO cells, while knockdown of mROS3 expression resulted in the decreased rate of cell migration (Figure 1). Immunoprecipitation and immunocytochemical analysis revealed that mROS3 interacted with P-type ATPase, a candidate enzyme responsible for the inward movement of aminophospholipids. mROS3 knockdown cells caused mislocalization of P-type ATPase and were defective in inward movement of fluorescence-labeled analogs of aminophospholipids across the plasma membrane. These results suggest that one of the cellular functions of mROS3 is serving as an escort protein that is required for the proper localization of P-type ATPase, and that organized movement of phospholipids plays an important role in regulation of cell motility.

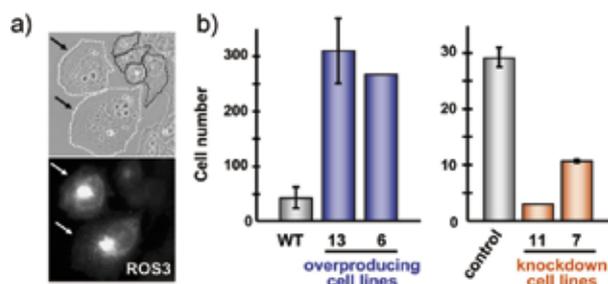


Figure 1. Expression levels of mROS3 protein affected cell morphology and cell motility in CHO cells. a) Wild CHO cells (a black line) and mROS3 overproducing cells (arrows, a white line). b) Migration of mROS3 overproducing or knockdown cells was studied by transwell assay and was quantitated by counting cells migrating across the membrane after 3h.

Role for Dystroglycan in Ca^{2+} -mediated Regulation of Mitochondrial Oxidative Phosphorylation and Behavioral Thermoregulation of *Drosophila*

Both ectothermic and endothermic animals move towards thermally comfortable zones, spending most of time at their preferred environmental temperatures. Considerable progress has been made in the identification of molecules involved in the peripheral thermal sensation, but the molecular mechanisms underlying temperature preference remain poorly understood. Here we identify a new *Drosophila* mutant that exhibits a preference for extremely low temperatures, named *atsugari* (*atu*). We show that the cryophilic phenotype of the *atu* mutant is caused by the reduced expression of the *Drosophila* orthologue of dystroglycan (DmDG), a membrane glycoprotein that forms the core of dystrophin-glycoprotein complex. The cryophilic phenotype is rescued by ectopic expression of DmDG and is reproduced by the RNA interference-mediated suppression of the DmDG expression in wild-type flies. The reduced expression of DmDG causes sustained increase in the concentration of intracellular Ca^{2+} and activation of pyruvate dehydrogenase, a key enzyme involved in mitochondrial energy metabolism, resulting in a marked increase in metabolic rate and ATP synthesis (Figure 2). The cryophilic phenotype of the *atu* mutant is reversed completely by brief exposure to hyperoxic conditions, suggesting that the insufficient supply of oxygen for the activated mitochondrial oxidative phosphorylation lowers the set point for temperature preference. This study reveals a novel role for dystroglycan in the control of energy homeostasis and behavioral thermoregulation of *Drosophila*, which is critical for the adaptability of ectothermic animals to their respective thermal environments.

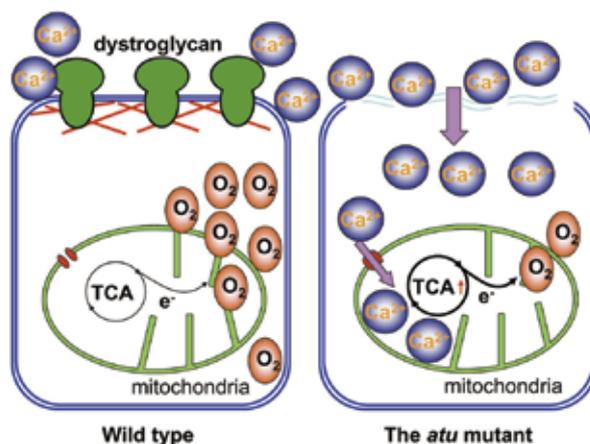


Figure 2. Dystroglycan plays a crucial role in the maintenance of energy homeostasis via intracellular Ca^{2+} handling, which is closely linked to thermoregulation in *Drosophila*.

Advanced Research Center for Beam Science - Particle Beam Science -

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Joint Institute for Nuclear Research, Russia, 21 January–11 February 2006
Joint Institute for Nuclear Research, Russia, 4–10 June 2006
Forschungszentrum Jülich, Germany, 4–10 June 2006
Lawrence Berkeley National Laboratory, USA, 1 November 2006
P. N. Lebedev Physical Institute, Russia, 20 November 2006

Scope of Research

The following subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Electron cooling of a hot proton beam; Compression of the energy spread of laser produced ion beams by an rf cavity for phase rotation; Research and development of permanent quadrupole magnets for final focusing of International Linear Collider (ILC); Generation of ultra-cold ion beams by electron and laser coolings; Mitigation of power loss due to skin effect.

Research Activities (Year 2006)

Presentations

Experimental Strategy for Realization of 3-D Beam Ordering with Use of Tapered Cooling at S-LSR, Noda A, Invited Talk at 39th ICFA Advanced Beam Dynamics Workshop, High Intensity High Brightness Hadron Beams, 31 May.

Commissioning of Electron Beam Cooling at S-LSR, Shirai T, 39th ICFA Advanced Beam Dynamics Workshop on High Intensity High Brightness Hadron Beams, 31 May.

High-energy High Frequency Buncher, Iwashita Y, 7th International Workshop on Neutrino Factories & Superbeams, 28 August.

Limits of RF Deflectors, Iwashita Y, Workshop on “ILC Small Crossing-angle Interaction Region”, 19 October.

Permanent Magnets, Iwashita Y, Workshop on “ILC Small Crossing-angle Interaction Region”, 20 October.

Grants

Noda A, Beam Accumulation and Cooler Ring, Advanced Compact Accelerator Research Project, Ministry of Education, Culture, Sports, Science and Technology, 1 April 2001–31 March 2006.

Iwashita Y, Super Strong Permanent Magnet for Final Focus Lens in Linear Collider, Grant-in-Aid for Scientific Research, (A) (1), 1 April 2002–31 March 2006.

Shirai T, High Energy Electron Extraction from Electron Storage Ring, Grant-in-Aid for Scientific Research, (C) (2), 1 April 2004–31 March 2006.

Beam Ordering of 7 MeV Protons at S-LSR

Charged particle beams are usually in the gas phase. Each particle has a large kinetic (thermal) energy in the particle rest frame. When the gas is cooled, it transfers to the liquid or solid state. When the charged particle beam is cooled, it is also predicted to move to the ordered state by phase transition. In the experimental studies, one dimensional transitions of the highly charged ions were found at GSI and MSI but it was not yet found for the single charged ions.

We carried out the electron cooling experiment of 7 MeV protons with the ion storage ring, S-LSR at ICR. The proton beam was cooled by electrons, which moved along protons in parallel and removed the thermal energy through a Coulomb interaction (see Figure 1). The result is shown in Figure 2 [1]. When the stored particle number was reduced, the space charge heating became weak and the momentum spread ($\propto \sqrt{T_{//}}$) was decreased. Around the particle number of a few thousands, the momentum spread dropped abruptly, which showed that the beam phase was changed and the space charge heating disappeared. The beam temperature changed from 3 K to 0.3 K.

[1] Noda A, Ikegami M, Shirai T, *New J. Physics*, **8**, 288 (2006).

Real-time Observation of Laser Produced Ions

Recently there are many reports of high energy ions produced by intense ultra-short-pulse lasers. For the production of energetic ions by irradiating an intense laser on a foil target, the optimization of the various conditions is required. So far the energy spectrum of ions has been detected by a solid-state track detector so-called CR-39. The data analysis with the CR-39, however needs a longer time. Therefore, the real-time adjustment of the experimental parameters has been difficult.

The energy of ions can be obtained by the time-of-flight (TOF) from the production target. We have succeeded to extract the TOF signals of protons under the backgrounds due to the high power laser using a plastic scintillation

counter shielded by special filters. By using the TOF detector, the energy spectrum as shown in Figure 3, can be obtained with real time.



Figure 1. View of the electron cooler at S-LSR.

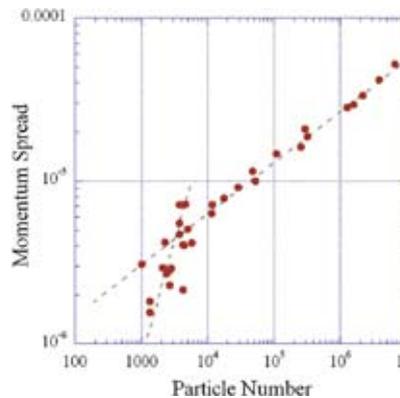


Figure 2. Dependence of momentum spread of protons on the particle number with the electron current of 25 mA at the cooler.

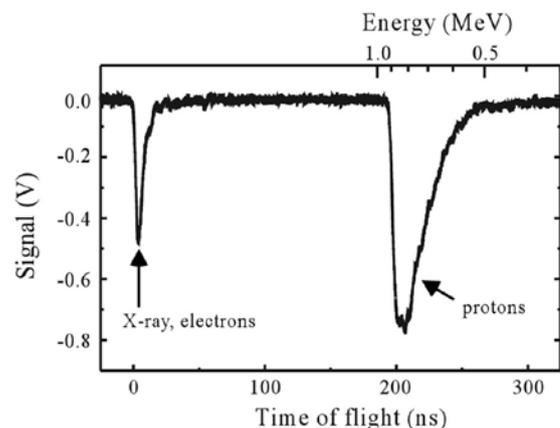


Figure 3. Typical TOF signal of protons obtained by photomultiplier. The protons are produced by a Ti:sapphire laser system called JLITE-X at JAEA Kansai Photon Science Institute.

Noda A, Design of Accelerator Systems for Compact On-site Neutron Sources, Synthetic Support Project for Accelerator Science, 8 July 2005–31 March 2006.

Iwashita Y, Research of Problems with High-Gradient Field ILC Superconducting rf Cavity, Joint Development Research at High Energy Accelerator Research Organization (KEK), 1 April 2005–31 March 2006.

Iwashita Y, Application and Development of Super

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

Award

Fadil H, PASJ Award for Young Scientists, Proof of Electron Cooling of Hot Ion Beams, Particle Accelerator Society of Japan, 4 August 2006.

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

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



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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 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-ray 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 2006)

Presentations

High-average-power, High-efficient Operation of Q-switched Cryogenic Yb:YAG Laser, Tokita S, Kawanaka J, Fujita M, Kawashima T, Izawa Y, Advanced Solid-State Photonics 2006 (OSA), January, Nevada, USA.

High-energy Pico-second Regenerative Amplifier with Cryogenically Cooled Yb:YAG, Tokita S, Kawanaka J, Fujita M, Kawashima K, Izawa Y, The Conference on Lasers and Electro-Optics 2006 (IEEE and OSA), May, California, USA.

The Processing of Single Crystal Diamond by Ultra-short Pulse Laser, Harano K, Nakamae K, Toda N, Hashida M, Shimizu S, and Sakabe S, 4th International Congress on Laser Advanced Materials Processing, 16–19 May, Kyoto, Japan.

Nano-ablation with an Intense Femto-second Laser, Hashida M, Shimizu S, Sakabe S, Canada-Japan SRO-COAST Symposium on Ultrafast Intense Laser Science 1, 7–8 July, Tokyo, Japan.

Terahertz Radiation from Argon Gas Jet Excited with Intense Femto-second Laser Pulses, Nagashima N, Shibuya K, Hangyo M, Hashida M, Sakabe S, Joint 31st International Conference on Infrared and Millimeter Waves and 14th International Conference on Terahertz Electronics (IRMMW-THz2006), 18–22 September, Shanghai, China.

Femto-second Laser Ablation of Carbon-nanotube Cathode, Hashida M, Shimizu S, Sakabe S, 5th Asia Pacific Laser Symposium (APLS2006), 23–27 November, Guilin, China (Invited).

Intense Femto-second Laser-Cluster Interaction, Sakabe S, Hashida M, Shimizu S, Masuno S, 5th Asia Pacific Laser Symposium (APLS2006), 23–27 November, Guilin, China (Invited).

Terahertz Radiation from Argon Clusters Irradiated by Intense Femto-second Laser Pulses, Nagashima N, Shibuya K, Hangyo M, Hashida M, Sakabe S, 5th Asia Pacific Laser Symposium (APLS2006), 23–27 November, Guilin, China.

Grants

Sakabe S, Fundamental Research on γ -ray Laser with Intense Femto-second Lasers, Grant-in-Aid for Scientific Research (A), 1 April 2006–31 March 2009.

Hashida M, Advanced Material Processing with Femto-second Lasers, Grant-in-Aid for Young Scientists (B), 1 April 2005–31 March 2006.

Awards

Tokita S, The Best Oral Presentation Award: High-average-power, High-efficient Operation of Q-Switched Cryogenic Yb:YAG Laser, The Review of Laser Engi-

Skinning of Argon Clusters by Coulomb Explosion Induced with an Intense Femto-second Laser Pulse

The energy distributions of ions emitted from argon clusters Coulomb exploded at an intensity of $< 10^{17}$ W/cm² with an intense femto-second laser have been experimentally studied. The power m of energy E of the ion energy distribution ($dN/dE \sim E^m$) is expected to be 1/2 for spherical ion clusters, but it is in fact reduced smaller than 1/2 as the laser intensity is decreased. This reduction can be well interpreted as resulting from the instantaneous ionization of the surface of the cluster. The validity of this interpretation was confirmed by experiments with double pulse irradiation. A cluster irradiated by the first pulse survives as a skinned cluster, and remaining core part is Coulomb exploded by the second pulse. It is shown that a cluster can be skinned by an intense short laser pulse, and the laser-intensity dependence of the skinned layer thickness can be reasonably explained by the laser-induced space charge field created in the cluster.

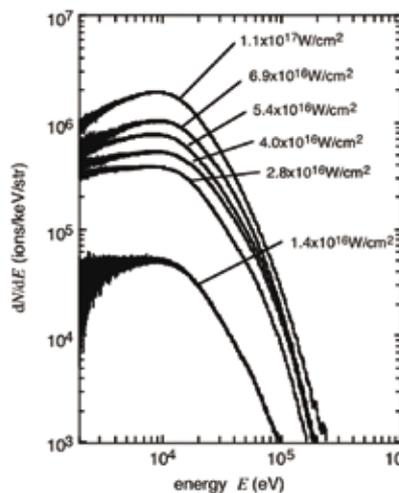
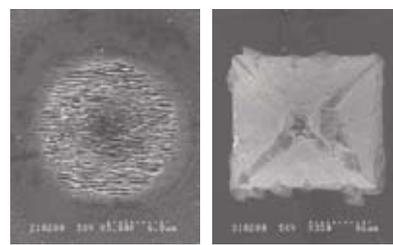


Figure 1. Energy distributions of Ar ions emitted from Coulomb-exploded Ar clusters, depending laser intensity. Backing pressure is 6 MPa.

Ultrashort Pulse Laser Ablation of Single Crystal Diamond

The laser ablation experiments on a single crystal diamond were carried out with a T6 laser (800 nm wavelength, 130 fs–400 ps pulse width). The ablation rate and the ablation threshold dependence on laser pulse width were investigated. The ablation threshold was found to be approximately proportional to pulse width to the power

0.34. It was suggested that the multi photon absorption was not predominated at this range of pulse width (166 fs–2 ps). The released ions upon the ablation process were studied by time-of-flight mass spectrometer (TOF-mass) with a 130 fs pulse laser. The TOF-mass spectra analysis revealed that the multi photon ionization is occurred, and the ablation mechanism are different at near the ionizing threshold energy from at the higher energy regime where thermal affect is predominant. These results indicate that the thermal effect is negligible at near the threshold energy, arising with laser energy at 130 fs laser ablation. The results of Raman spectra measurement suggested the possibility of the laser processing without thermal damage.



(a) 1.18ps, 0.97 J/cm² (b) 400ps, 0.7 J/cm²

Figure 2. SEM photographs of diamond surface ablated by 1000 pulses.

Development of High-average-power Pico-second Lasers with Cryogenically-Cooled Yb:YAG Crystal

Compact picosecond lasers with high average power are in high demand for precision micromachining. Cryogenically-cooled Yb:YAG crystal is one of the promising laser materials for the high-average-power picosecond lasers, because the cryogenically cooling takes advantage of significant improvement of the crystal's thermal properties at low temperatures such as higher thermal conductivity, lower thermo-optic coefficient, and lower thermal expansion coefficient. We have developed a diode-pumped picosecond 8-pass amplifier with a liquid-nitrogen-cooled Yb:YAG crystal. An average output power of 23.7 W with a near-diffraction-limited beam quality was obtained at a pulse repetition rate of 80 kHz and a pulse duration of 11.7 ps. This is the highest average power, to the best of our knowledge, obtained by single-stage diode-pumped ultrafast amplifiers with pulse energies above multi-hundreds of micro-joules. Average powers above 20 W were also obtained in the 30–80 kHz repetition rate range. The pulse energy reached almost 1 mJ at the 20 kHz repetition rate.

neering, May 2006.

Tokita S, Encouragement Prize for Oral Presentation, Research, High-energy Pico-second Regenerative Amplifier

with Cryogenically Cooled Yb:YAG, The Japan Society of Applied Physics, August 2006.

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

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National Tsing-Hua University, Taiwan, 1 September 2005–30 April 2006
McGill University, Canada, 23 August 2006
Nion, USA, 11 September 2006
University of Bristol, UK, 12 September 2006
National Taiwan University, Republic of China, 2 June 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 2006)

Presentations

Interpretation of Electron Energy-Loss Near-Edge Structure by First Principles Band Structure Calculation, Kurata H, Tsujimoto M, Nemoto T, Isoda S, The 3rd Japan-China Joint Seminar on Atomic Level Characterization, 6–10 March, Xiamen, China.

STM and STS Study on Platinum Chains in Bis(1,2-benzoquinonedioximate)platinum, Yaji T, Yoshida K, Tsujimoto M, et al., IMC16, 3–8 September, Sapporo,

Japan.

Atomic Resolution HAADF-STEM Analysis of Layered Double Perovskites $\text{La}_2\text{CuSnO}_6$, Haruta M, Masuno A, Kan D, et al., IMC16, 3–8 September, Sapporo, Japan.

Development of Cold-FEG with a Nanotip for 200kV TEM/STEM, Kurata H, Isoda S, Tomita T (JAERI), IMC16, 3–8 September, Sapporo, Japan.

Temperature and Electric Field Dependences of the Mobility of a Single-grain Pentacene Field-effect Transis-

Nanodiffraction and Characterization of Titanate Nanotube Prepared by Hydrothermal Method

Titanate nanotubes have been of great interest recently due to their potential application to dye sensitized solar cells, gas sensors and photocatalysts (Figure 1). Though the nanotubes are widely believed to be formed by rolling up sheet-like precursors, their detailed formation mechanism and crystal structure have been still under discussion. Therefore, we carefully investigated the local structure of a single nanotube as well as its co-product by using electron nanodiffraction technique. Titanate nanotubes were synthesized by a simple hydrothermal treatment of TiO_2 anatase powders. To observe the change of the diffraction pattern in the different small area, we focused a parallel electron probe as small as 1 nm in diameter and moved it across the nanotube (Figure 2). Our detailed local observations via electron nanodiffraction strongly suggest that the nanotubes are formed by rolling up the exfoliated lepidocrocite-type titanate sheet along the [100] direction without helicity.

Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor

A single-grain organic field-effect transistor (OFET) of pentacene with a $1 \mu\text{m}$ channel length of top-contact electrodes is demonstrated in a wide range of temperatures from 300 down to 5.8 K (Figure 3). No hysteresis behavior was observed in the transfer characteristics throughout the entire temperature range. The saturation mobility and on/off ratio are estimated as $1.11 \text{ cm}^2/\text{Vs}$ and 10^7 at 300 K and $0.34 \text{ cm}^2/\text{Vs}$ and 10^5 at 5.8 K, respectively. The non-monotonic temperature dependence of the mobility indicates a bandlike transport at high temperatures. The electric-field dependence of the mobility in the single-grain OFET does not show a Poole-Frenkel-like behavior. This indicates that Poole-Frenkel-like behavior observed in con-

ventional OFETs can be attributed to the disorder of molecules; single-grain OFET is free from such disorders.

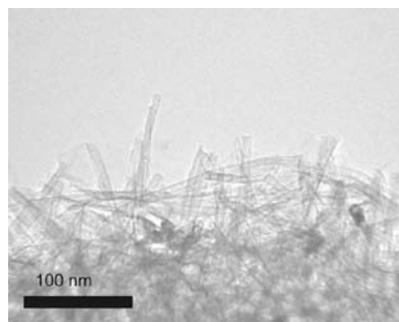


Figure 1. Typical TEM images of titanate nanotubes.

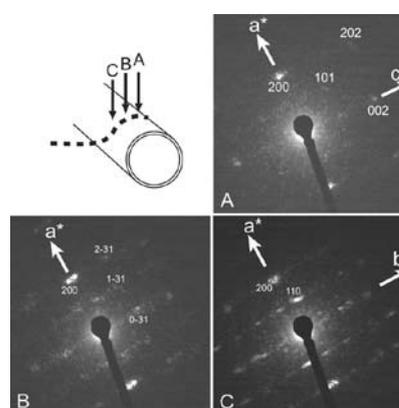


Figure 2. The incident electron beam was moved across the nanotubes from the center (A) to the side (C) of one nanotube.

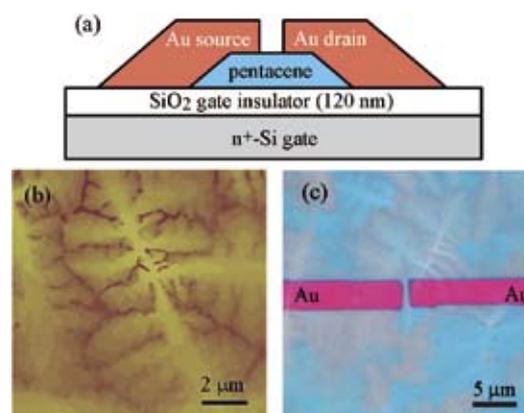


Figure 3. (a) Schematic cross section of a single-grain OFET with top-contact structure. (b) Morphology of vacuum-deposited pentacene film observed with an AFM. (c) Optical microscope image around a channel region of a single-grain OFET with $1 \mu\text{m}$ of channel length.

tor, Minari T, Nemoto T, Isoda S, Intern. Forum on Green Chem. Sci. & Eng. and Process Systems Engineering, 8–10 October, Tianjin, China.

Iron Oxides Nanostructure; Growth, Characterization and Applications, Chou L J, Lai M W (NTHU) et al., Nabisconference, 8–9 August 2006, Chicago, USA.

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 2006–31 March 2007.

Advanced Research Center for Beam Science - Structural Molecular Biology -

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GODA, Yuko (M2)
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Visitors

Dr SHERMAN, Evgeeny Department of Physics, University of Toronto, Canada, 15–26 October 2006
Dr JULIEN, Christian Institut des Nanoscience de Paris, Universite Pierre et Marie Curie, France, 5–6 September 2006

Scope of Research

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

Research Activities (Year 2006)

Grants

Hata Y, Structural Analyses of Gene-products Involved in Protein Structure Formation, Protein 3000 Project, 1 April 2002–31 March 2006.

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.

Crystallographic Studies of Binding Mode of Protein I^C toward Carboxypeptidase Y

The protein I^C from *Saccharomyces cerevisiae* inhibits carboxypeptidase Y (CPY) by forming the 1:1 complex. We determined the 2.7 Å crystal structure of the I^C-CPY complex by X-ray crystallography to reveal the inhibitory mode of I^C against CPY (Figure 1).

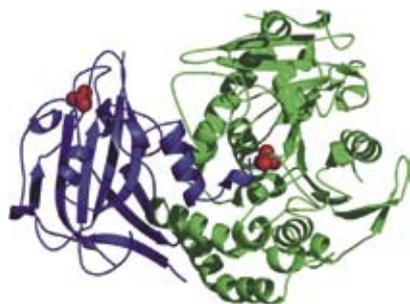


Figure 1. Ribbon drawing of the I^C-CPY complex at 2.7 Å resolution. I^C and CPY are shown in blue, green, respectively. Sulfate ions are represented by red spheres.

The structure of the I^C-CPY complex reveals that I^C binds to CPY with multiple-binding sites and that the N-terminal portion (Ac-Met11-Lys731) contains not only the N-terminal inhibitory reactive site (Figure 2a) but also a large portion of the secondary binding site (Figure 2b). In addition, the complex structure reveals that the specific binding of the N-terminal acetyl group to the active site of CPY is a novel proteinase-protein inhibitor interaction, and contributes to a tight interaction with CPY and to its complete inactivation.

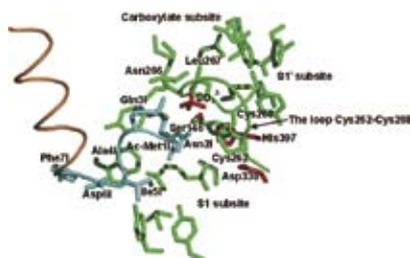


Figure 2a. Binding of the N-terminal inhibitory reactive site to the active site of CPY. The side-chains of residues that form the catalytic triad (red) and substrate-binding sites of CPY and the inhibitory reactive site of I^C are depicted as stick models.

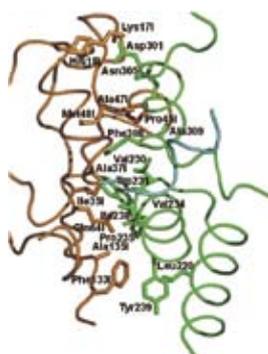


Figure 2b. The secondary binding site of I^C. The side-chains of residues involved in the interaction at the binding interface are depicted as stick models with labels.

To further clarify the proteinase-inhibition mode of I^C indicated by the three-dimensional structure of the complex with CPY, we analyzed the biochemical properties of various I^C mutants: the N-terminal unacetylated form (unal^C), the N-terminal modified form in which Gly is added to the N-terminus to mimic the acetyl group (gl^C), the N-terminal deleted form (d1-7I^C), and the unacetylated and C-terminal deleted form (d217-219I^C). Gel filtration chromatography of mixtures of the native and mutant inhibitors with CPY showed that I^C, unal^C, gl^C, and d217-219I^C produced single peaks in the position corresponding to the I^C-CPY complex but that the N-terminal deleted mutant (d1-7I^C) formed no complex with CPY (Figure 3).

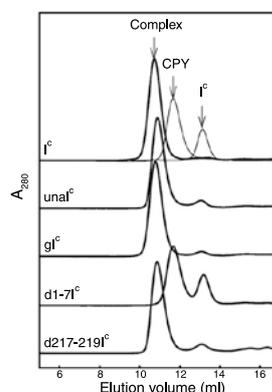


Figure 3. Gel filtration analysis of equimolar mixtures of the native and mutant forms of I^C with CPY. Thick lines, the mixtures; thin lines, free CPY and I^C used as the reference.

The majority of endoproteinase inhibitors and carboxypeptidase inhibitors, the three-dimensional structures of which were previously elucidated at atomic resolution, were directed toward their target proteinases so that they interact with the active sites of the proteinases in a substrate-like manner through an inhibitory reactive site alone. In contrast, the inhibition and interaction modes of I^C toward CPY have the three features that are different from those of the canonical inhibitors described above: (1) the masking of the active site of CPY in a non-substrate-like manner, (2) the involvement of the N-terminal acetyl group introduced posttranslationally in the complete inhibition of the proteinase, and (3) multiple-site binding to the proteinase. Thus, the binding of I^C toward CPY is the prototype of a novel class of proteinase-protein inhibitor interactions. Furthermore, considering the loss of the binding affinity of the N-terminal deleted mutant (d1-7I^C) to CPY (Figure 3), it is reasonable to assume that I^C firstly binds to CPY via the inhibitory reactive site alone, and then the secondary CPY-binding site come into contact with the enzyme to form the stable complex between the proteins.

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Scope of Research

Depletion of fossil and rare metal resources, which the chemical industry relies on, is crucial problem for human society. Our research activity is devoted to the discovery, design and development of new molecular transformation reactions that enable efficient exploitation of chemical resources, such as unsaturated hydrocarbons, haloalkanes, etc. The present research subjects are (1) a substitution reaction of unreactive haloalkanes with various organometallic compounds promoted by feedstock metals such as iron, zinc, and magnesium (2) understanding and design of synergetic effects of multi-metallic centers on the catalysis by the use of quantum chemistry.

Research Activities (Year 2006)

Presentations

Development of New Organometallic Substitution Reactions toward Exploitation of Chemical Resources, Nakamura M, 1st European Chemistry Congress, Budapest, Hungary, 27–31 August 2006.

Iron-Catalyzed Cross Coupling of Haloalkanes, Ito S, Nakamura M, 1st International Conference on Cutting-Edge Organic Chemistry in Asia Tiruru, Naha, Okinawa, Japan, 16–20 October 2006.

Cross Coupling of Haloalkanes under Iron Catalysis, Nakamura M, 98th Catalysis Society of Japan Meeting, Toyama, Japan, 26–29 September 2006.

Grants

Nakamura M, Development of Iron Catalyzed Reaction for Transformation of Polyvinylchloride, Grant-in-Aid for Exploratory Research, 1 April 2005–31 March 2007.

Nakamura M, Molecular Transformation of Unreactive Haloalkanes, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2007.

Nakamura M, Design and Application for Methodology

of Multi-Metallic, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2006–31 March 2010.

Hatakeyama T, Development of SN2 Reaction of Carbon-Heteroatom Bond with Highly Reactive Metal Enolate, Grant-in-Aid for Young Scientists (Start), 1 April 2006–31 March 2008.

Awards

Nakamura M, Lectureship Award to China, 1st International Conference on Cutting-Edge Organic Chemistry in Asia, 20 October 2006.

Nakamura M, Lectureship Award to Hong Kong, 1st International Conference on Cutting-Edge Organic Chemistry in Asia, 20 October 2006.

Nakamura M, Banyu Young Chemist Award 2006, Banyu Life Science Foundation International, 18 November 2006.

Hatakeyama T, Kaneka Award in Synthetic Organic Chemistry, The Society of Synthetic Organic Chemistry, Japan, 30 November 2006.

Iron Catalyzed Cross-Coupling Reaction

Chloroalkanes, derived from olefins in one step, are feedstock carbon resources in industry. However, there are few methods to transform C–Cl bond into C–C bond directly under mild conditions due to its chemical stability. We have developed several iron-catalyzed C–C bond formation reactions, enantioselective olefin carbometalation reaction and diastereoselective addition/ring-opening reaction. Recently, we found cross-coupling reaction of haloalkanes and aryl magnesium compounds takes place in the presence of FeCl_3 and N, N, N', N' -tetramethylethylenediamine (TMEDA). Under these conditions, even secondary alkyl chlorides, known to be unreactive substrate for substitution reaction, gave coupling products in up to 99% yield. The use of aryl zinc compounds, which shows mild nucleophilicity and basicity, enable to introduce functional groups such as ester and nitrile on the alkyl and/or aryl moieties.



Figure 1. Iron-Catalyzed Cross-Coupling Reaction.

The liquid crystal (LC) molecules used for active matrices LC displays, such as TV, PC, and portable phones, widely have a fluoroaryl cyclohexane substructure as a mesogen moiety. As shown in Figure 1, iron catalyzed cross-coupling reaction of functionalized aryl zinc compounds and chlorocyclohexanes (or bromocyclohexanes) can construct the phenylcyclohexane skeleton in shorter steps from cheaper starting materials than the present industrial methods (9 steps), which consume expensive and toxic transition metal catalysts, such as palladium and nickel.

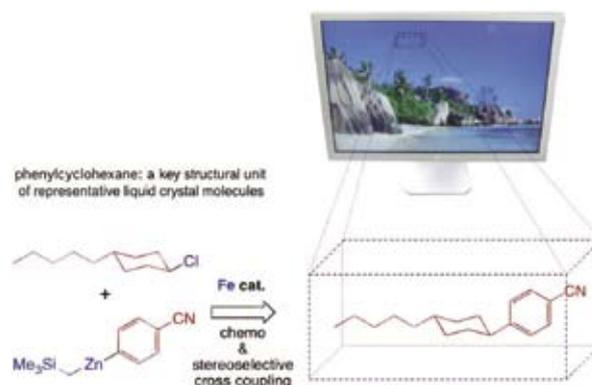


Figure 2. Facile synthesis of liquid crystal molecules.

SN2 Reaction of Haloalkanes with Magnesium Enamides

SN₂-type substitution reaction at asymmetric carbon center, yielding Walden inversion product, is known to be a powerful tool in controlled organic synthesis. However, it is difficult to carry out SN₂ reaction with carbon nucleophiles due to its sterical hindrance and considerable basicity. Recently, we found that magnesium enamide, possessing chelate structure, is highly nucleophilic and moderately basic to substitute secondary haloalkanes. It is noteworthy that unreactive haloalkanes, fluoro- and chloroalkanes smoothly react with magnesium enamide to provide α -alkylated ketones in up to 97% yield upon hydrolysis of imine moiety and optically active chloroalkanes give the corresponding “Walden inversion” adduct with high enantioselectivity.

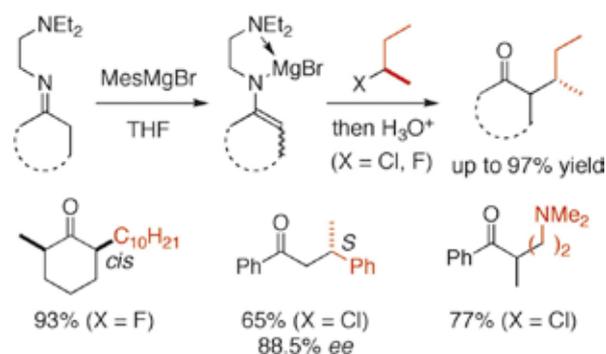


Figure 3. SN₂ Substitution Reaction of Fluoro- and Chloroalkanes.

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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 2006)

Presentations

Magnetic Structure of $\text{SrCo}_6\text{O}_{11}$ with Magnetization Plateau, Saito T, Takeda Y, Williams A, Atfield P, Wuernisha T, Kamiyama T, Ishiwata S, Shimakawa Y, Takano T, 61st Annual Meeting, The Physical Society of Japan, 27–30 March (Matsuyama).

Neutron Diffraction Study of a Layered Cobalt Oxide $\text{SrCo}_6\text{O}_{11}$, Saito T, Williams A, Atfield P, Wuernisha T, Kamiyama T, Ishiwata S, Takeda Y, Shimakawa Y, Takano M, 17th International Conference on Magnetism, 20–25 August (Kyoto).

Spin Frustration in $\text{SrCo}_6\text{O}_{11}$, Saito T, Williams A, Atfield P, Wuernisha T, Kamiyama T, Ishiwata S, Takeda Y, Shimakawa Y, Takano M, Kyoto Conference on Solid State Chemistry, 14–18 November (Kyoto).

Single Crystal Growth of Calcium Oxychloride Superconductors $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ and $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$ at High Pressure, Yamada I, Azuma M, Ohish K, Shimakawa Y, Takano M, Kyoto Conference on Solid State Chemistry, 14–18 November (Kyoto).

Synthesis and Magnetic Properties of $L1_0$ -FePt Nanoparticles, Yamamoto S, Morimoto Y, Tamada Y, Takahashi Y K, Hono K, Ono T, Takano M, Kyoto Conference on Solid State Chemistry, 14–18 November (Kyoto).

Synthesis, Structural and Physical Properties of A-site

Cation Deficient Single Layer Oxychloride Superconductor $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$, Yamada I, Azuma M, Belik A, Harjo S, Kamiyama T, Shimakawa Y, Takano M, 8th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductor, 9–14 July (Dresden).

High Pressure Single Crystals Growth of Calcium Oxychloride Superconductors, Yamada I, Azuma M, Shimakawa Y, Takano M, Fall Meeting 2006, The Physical Society of Japan, 23–26 Fall (Chiba).

Preparation of $L1_0$ -FePt Nanoparticles Dispersible in Nonpolar Organic Solvents, Yamamoto S, Morimoto Y, Tamada Y, Takahashi Y K, Hono K, Ono T, Takano M, The 30th Annual Conference on Magnetism in Japan, 11–14 September (Shimane).

Blue-light Emission at Room Temperature from Ar^+ -irradiated SrTiO_3 , Kan D, Terashima T, Kanda R, Masuno A, Ishizumi A, Kanemitsu Y, Shimakawa Y, Takano M, APS March Meeting 13–17 March (Baltimore).

Blue Luminescence at Room Temperature from Electron-doped SrTiO_3 , Kan D, Kanda R, Masuno A, Terashima T, Ishizumi A, Kanemitsu Y, Shimakawa Y, Takano M, The 53rd Spring Meeting, 2006; The Japan Society of Applied Physics and Related Societies, 22–26 March (Tokyo).

SrCo₆O₁₁ with Anomalous Magnetotransport Property

SrCo₆O₁₁ is a layered cobalt oxide with anomalous magnetoresistance, first synthesized using a high pressure technique in our group. It was found that SrCo₆O₁₁ comprises itinerant electrons and Ising-like local spins of $S = 2$ on separate crystallographic sites, having strong interactions with each other. The spin structure at the 1/3 magnetization plateau state was found to be ferromagnetic in the ab -plane and like $\uparrow\text{-}\uparrow\text{-}\downarrow\text{-}\uparrow\text{-}\uparrow\text{-}\downarrow$ along the c -axis. The quick reorientation of the ferromagnetic layers from the $\uparrow\text{-}\uparrow\text{-}\downarrow$ ($M/M_0 = 1/3$; M_0 = saturated magnetization) manner to the $\uparrow\text{-}\uparrow\text{-}\uparrow$ ($M/M_0 = 1$) manner under magnetic field should result in a major change of the magnetic scattering of conduction electrons penetrating through the ferromagnetic layers, which explains the negative, sharp and two-stepped magnetoresistance.

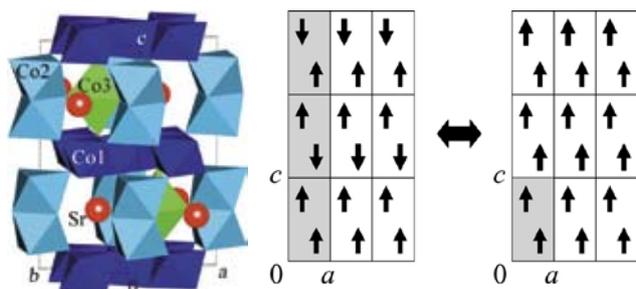


Figure 1. The crystal structure and spin structures of SrCo₆O₁₁.

Monodisperse and Highly Coercive L1₀-FePt Nanoparticles Dispersible in Nonpolar Organic Solvents

The FePt alloy with the L1₀ structure possesses a very high uniaxial magnetic anisotropy of ca. 6×10^6 J/m³, which is more than ten times as high as that of the currently utilized CoCr-based alloys. Superparamagnetic fluctuation of the room temperature magnetization can

thus be suppressed even for particles of 3 nm in diameter, making an appropriate array of these nanoparticles to be a promising candidate for future ultra-high density magnetic recording media of >1 Tbit/inch². The most basic requisite for the practical use would be the formation and the fixation of an array on a substrate with the magnetic easy axis, *i.e.*, the tetragonal c axis, oriented normal to the substrate surface. Such a close packed triangular array structure may be formed through self-organization under an external magnetic field if the L1₀-FePt nanoparticles could be dispersed in a polymer binder. We developed a method to prepare monodisperse and highly coercive L1₀-FePt nanoparticles which are dispersible in nonpolar organic solvents such as toluene, chloroform, and hexane. By vigorously stirring the SiO₂-coated L1₀-FePt nanoparticles synthesized by the “SiO₂-nanoreactor” method (*Appl. Phys. Lett.* **2005**, *87*, 032503) in a mixture of an aqueous NaOH solution, chloroform, and hexadecyltrimethylammonium bromide, the SiO₂ coating was dissolved off and bare FePt nanoparticles could be extracted to the chloroform phase without degrading their magnetic properties. The present success may promote the practical application to ultra-high density magnetic recording and also may open the door to providing these particles with new physical and/or chemical functions.

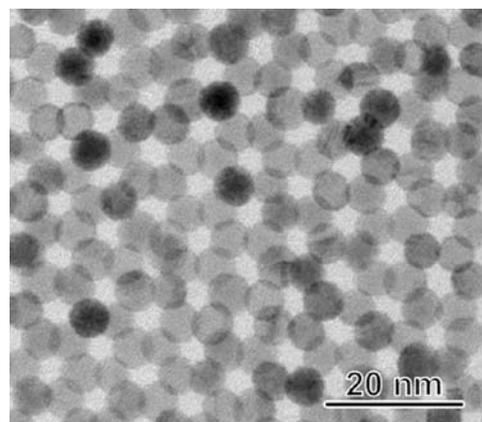


Figure 2. TEM image of the L1₀-FePt nanoparticles.

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.

Award

Yamamoto S, MSJ Outstanding Presentation Award, The 30th Annual Conference on Magnetism in Japan, “Preparation of L1₀-FePt Nanoparticles Dispersible in Nonpolar Organic Solvents,” The Magnetism Society of Japan, 22 November 2006.

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Scope of Research

This laboratory aims at establishment of new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using kinetic techniques on the reaction intermediates and elementary processes. The research subjects include: (1) development of novel ligand systems for catalysis, (2) creation of functional metal complexes based on synergistic effects, (3) construction of π -conjugation system including transition-metals, and (4) development of functional molecules including transition-metal clusters.

Research Activities (Year 2006)

Presentations

Studies on Introduction of Functional Groups onto the [4Fe-4C] Cluster: Application for Construction of Functional Molecules Containing Transition-metal Clusters, Okazaki M, 21st Century COE on Kyoto University Alliance for Chemistry "The 3rd Organoelement Chemistry Seminar", 26 October, Kyoto, Japan.

Introduction of Functional Groups onto the Fe₄C₄ Clusters, Okazaki M, 2006 Workshop on Organometallic Chemistry, 1–2 December, Kyoto, Japan.

Synthesis of Haloacetylene- and Dihaloacetylene-Coordinated Tetrairon Clusters and Their Reactivities toward Nucleophiles, Yoshimura K, Uehira K, Takano M, Okazaki M, Ozawa F, 53rd Symposium on Organometallic Chemistry, 8 September, Osaka, Japan.

π -Conjugated Organometallic Complexes with Highly Efficient $d\pi$ - $p\pi$ Interaction between Platinum and sp^2 -Hybridized Phosphorus Ligand, Ozawa F, Hayashi K, Nakatani M, Okazaki M, Toyota K, Yoshifuji M, XXII International Conference on Organometallic Chemistry (ICOMC 2006), 23–28 July, Zaragoza, Spain.

Diphosphinidene-cyclobutene-coordinated Complexes: Structures and Catalysis, Ozawa F, The 3rd RIKEN Symposium on the Frontiers of Organometallic Chemistry, 6

October, Wako, Japan (Invited).

Stereocontrolled Synthesis and Optical Properties of All-cis Poly(arylene vinylene)s, Ozawa F, Lectureship of the Chemistry Research Promotion Center, National Science Council, Republic of China, 8 November, Institute of Chemistry, Academia Sinica, Taipei, Taiwan (Invited).

Highly Active Catalysts Bearing Diphosphinidene-cyclobutene Ligands (DPCB), Ozawa F, Lectureship of the Chemistry Research Promotion Center, National Science Council, Republic of China, 9–10 November, National Tsing Hua University, Hsinchu, and National Taiwan University, Taipei, Taiwan (Invited).

Grants

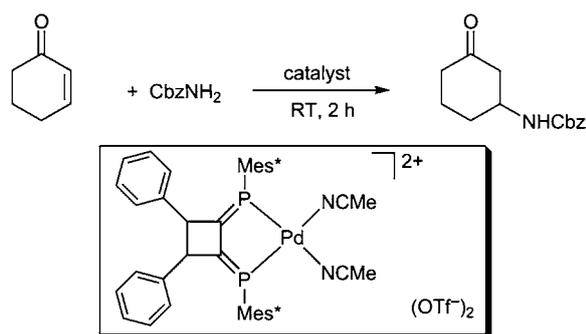
Okazaki M, Chemistry of "Ethyne Cation"-Coordinated Transition-Metal Clusters, Grant-in-Aid for Young Scientists (B), April 2005–March 2007.

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

Ozawa F, Creation and Applications of Acidic Transition Metal Hydrides, Grant-in-Aid for Priority Area "Advanced Molecular Transformations", April 2006–March 2007.

Synthesis and Catalytic Properties of Cationic Palladium(II) and Rhodium(I) Complexes Bearing Diphosphinidene-cyclobutene Ligands

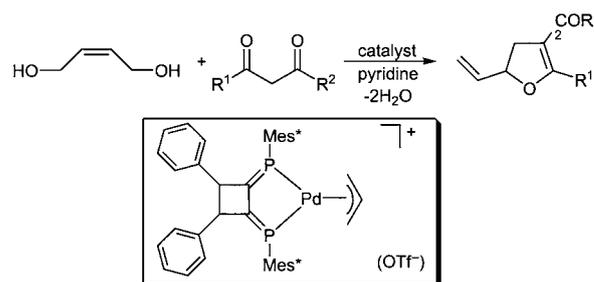
Cationic palladium(II) and rhodium(I) complexes bearing 1,2-diaryl-3,4-bis[(2,4,6-tri-*t*-butylphenyl)phosphinidene]cyclobutene ligands (DPCB-Y) were prepared and their structures and catalytic activity were examined (aryl = phenyl (DPCB), 4-methoxyphenyl (DPCB-OMe), 4-(trifluoromethyl)phenyl (DPCB-CF₃)). The palladium complexes [Pd(MeCN)₂(DPCB-Y)]X₂ (X = OTf, BF₄, BAr₄ (Ar = 3,5-bis(trifluoromethyl)phenyl)) were prepared by the reactions of DPCB-Y with [Pd(MeCN)₄]X₂, which were generated from Pd(OAc)₂ and HX in MeCN. On the other hand, the rhodium complexes [Rh(MeCN)₂(DPCB-Y)]OTf were prepared by the treatment of [Rh(μ-Cl)(cyclooctene)₂] with DPCB-Y in CH₂Cl₂, followed by treatment with AgOTf in the presence of MeCN. The cationic complexes catalyzed conjugate addition of benzyl carbamate to α,β-unsaturated ketones.



Scheme 1. Hydroamidation of enones with CbzNH₂ catalyzed by DPCB-Pd complex.

Cyclodehydration of *cis*-2-Butene-1,4-diol with Active Methylene Compounds Catalyzed by a Diphosphinidene-cyclobutene-coordinated Palladium Complex

The palladium-catalyzed allylation is a useful synthetic means of constructing C-C, C-N, and C-O bonds. (π -Allyl)palladium triflate coordinated with 1,2-bis(4-methoxyphenyl)-3,4-bis(2,4,6-tri-*t*-butylphenylphosphinidene)cyclobutene (DPCB-OMe), [Pd(η^3 -C₃H₅)(DPCB-OMe)]OTf, efficiently catalyzes cyclodehydration of *cis*-2-butene-1,4-diol with active methylene compounds such as acetylacetone and ethyl acetoacetate in toluene in the presence of pyridine. The reactions can be performed in air, giving 2-vinyl-2,3-dihydrofurans in good to high yields.



Scheme 2. Cyclodehydration of *cis*-2-butene-1,4-diol with acetylacetone catalyzed by DPCB-Pd complex and pyridine.

Redox-Induced Recombination of C-C Bonds on Fe₄ Framework

Metal clusters have recently attracted much attention due to their rich redox properties. We previously reported the syntheses of [Cp'₄Fe₄(HCCH)(HCCR)]⁺ (Cp' = C₃H₄Me, R = alkyl, alkynyl, S^{*p*}Tol, PPh₂) via bromination of the HCCH moiety in [Cp'₄Fe₄(HCCH)₂]⁺, followed by nucleophilic substitution. Similarly, [Cp'₄Fe₄(HCCR)₂]⁺ (R = -C≡CSiMe₃, [1-anti]⁺) was obtained from the reaction of a dibromo-substituted cluster with HC≡CSiMe₃/CuI/NHEt₂. Interestingly, there is an equilibrium between [1-anti]⁺ and its isomer [Cp'₄Fe₄(HCCH)(RCCR)]⁺ ([1-syn]⁺). In contrast, transformation between their neutral forms was not observed. Oxidation of [1-anti]⁺ led to the exclusive formation of [Cp'₄Fe₄(HCCH)(μ₃-CR)₂]²⁺ ([2]²⁺) (Figure 1). Both structural changes should proceed through the intramolecular recombination of Fe-Fe and C-C bonds on the Fe₄C₄ core.

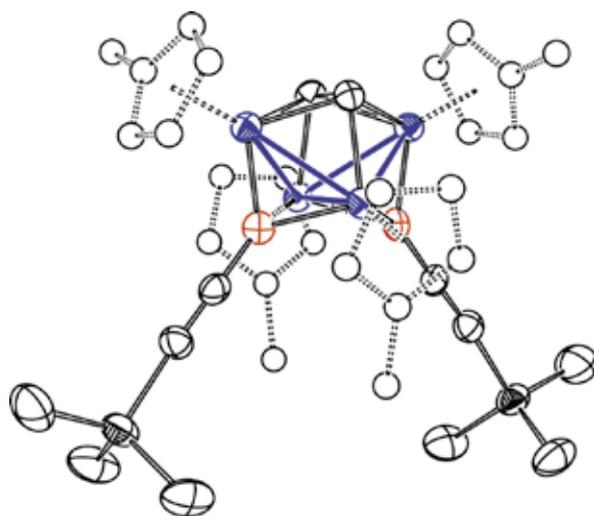


Figure 1. Molecular structure of [Cp'₄Fe₄(HCCH)(μ₃-C≡CSiMe₃)₂]²⁺ ([2]²⁺).

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Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-structured materials and to establish opto-nanoscience for creation of innovative functional materials. Optical properties of semiconductor quantum nanostructures and strongly-correlated electron systems in low-dimensional materials are studied by means of space- and time-resolved laser spectroscopy. The main subjects are as follows: (1) Investigation of optical properties of single nanostructures through the development of high-resolution 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 2006)

Presentations

Nanoimaging Spectroscopy and Its Application Using Near-Field Scanning Optical Microscope (Invited), Matsuda K, The General Meeting of Kansai Branch of the Japanese Society of Microscopy, 22 July 2006, Kyoto, Japan.

Exciton Luminescence of Single-walled Carbon Nanotubes Investigated by Single Nanotube Spectroscopy, Inoue T, Matsuda K, Murakami Y, Maruyama S, Kanemitsu Y, 28th International Conference on Physics of Semiconductor (ICPS28), 24–28 July 2006, Vienna, Austria.

Mechanism of Surface-Enhanced Light Emission from Single CdSe Nanoparticles on Metal Substrates, Ito Y, Matsuda K, Kanemitsu Y, 28th International Conference on Physics of Semiconductor (ICPS28), 24–28 July 2006, Vienna, Austria.

Photoluminescence Dynamics in Highly Excited GaN-based Ternary Alloys, Hirano D, Inouye H, Kanemitsu Y, 28th International Conference on Physics of Semiconductor (ICPS28), 24–28 July 2006, Vienna, Austria.

Grants

Kanemitsu Y, Basic Research for Development of Near-Field Optical Microscope for Elemental Analysis and Mass Spectrometry, Grant-in-Aid for Exploratory Re-

search, 1 April 2005–31 March 2007.

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

Matsuda K, 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, 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.

Matsuda K, Development of Near-Field Scanning Optical Microscope with Nanometer-Level Spatial Resolution, Research Foundation for Opt-Science and Technology, Research Grant, 1 April 2005–31 March 2007.

Inouye H, Luminescence Dynamics of Self-Assemble Nanocrystal Composite Film and Study for Realizing

Mechanism of Photoluminescence Enhancement in a Single CdSe Semiconductor Nanocrystal/Metal Interface

Colloidal semiconductor nanocrystals with high photoluminescence (PL) quantum efficiencies have been extensively studied both from the viewpoint of fundamental physics and with consideration for the potential applications to electronics and biotechnology. The interfaces between metals and nanocrystals play complex and essential roles in the optical responses of semiconductor nanocrystals on metals. The detailed understanding interactions between nanocrystals and metal surface are very important to enhance the PL intensity of nanocrystals in conjunction with the improvement of the PL efficiency of nanocrystals. We have studied the mechanism of the PL enhancement and quenching of single CdSe/ZnS core/shell nanocrystals on Au surfaces by means of single nanocrystal spectroscopy. The *on-off* PL blinking observed on the glass surface (upper panel of Figure 1) is drastically suppressed on Au surfaces (lower panel of Figure 1), because of the

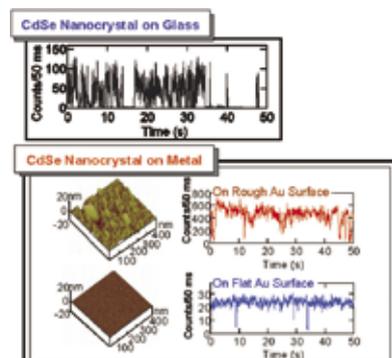


Figure 1. PL time-traces of a single CdSe/ZnS nanocrystal on glass and metal substrate.

fast energy transfer between Au surfaces and nanocrystals. The PL enhancement of single CdSe/ZnS nanocrystals occurs on rough Au surfaces, but PL quenching occurs on flat Au surfaces, compared to the case of the glass surface. Single nanocrystal spectroscopy reveals that the PL enhancement on rough Au surfaces is caused by the suppression of PL blinking and the electric field enhancement due to localized plasmon excitation.

High Luminescence Efficiency, Grant-in-Aid for Young Scientists (B), 1 April 2005–31 September 2006.

Awards

Kanemitsu Y, Pioneering and Outstanding Contributions to Nano-silicon Optoscience, Inoue Prize for Science, Inoue Foundation for Science, 3 February 2006.

Kanemitsu Y, Outstanding Contributions to Semicon-

Exciton-phonon Interaction in Individual Single-Walled Carbon Nanotubes Studied by Micro-Photoluminescence Spectroscopy

Electronic and optical properties of single-walled carbon nanotubes (SWNTs) have attracted much attention both from the fundamental physics viewpoint and due to the potential applications to opto-electronic devices. The recent discovery of efficient photoluminescence (PL) from isolated semiconducting SWNTs has stimulated considerable efforts in understanding optical properties of SWNTs. However, the SWNTs samples are usually inhomogeneous systems in the sense that many different species of nanotubes exist: the inhomogeneous broadening and the spectral overlapping of PL peaks cause the complicated spectra. It is therefore needed to perform PL measurements on single SWNTs for clarifying the optical properties of each SWNT species. Single nanotube spectroscopy provides us essential information such as exciton-phonon interaction. We have investigated the diameter dependence of the exciton luminescence linewidth in individual SWNTs by means of micro-photoluminescence (μ -PL) spectroscopy. The line-shapes of μ -PL spectra for single SWNTs suspended on a patterned Si substrate at room temperature can be fitted by single Lorentzian functions. The PL linewidth becomes broad in small diameter SWNTs. Our observation suggests that the exciton-phonon interaction becomes stronger with a decrease of the diameter, i.e., with an increase of the surface curvature. From the temperature dependence of the PL linewidth, it was found that the very low energy phonon mode has the dominant contribution to the diameter dependence of the linewidth broadening.

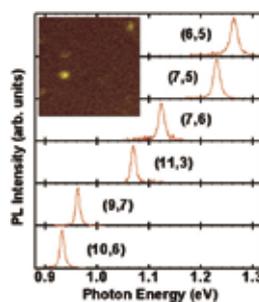


Figure 2. μ -PL spectra of single SWNTs with different chiral indices. Inset shows the PL image [7.6 μ m \times 7.6 μ m].

ductor Nanoparticle Optoscience, Yazaki Memorial Foundation Award, Yazaki Foundation, 9 March 2006.

Matsuda K, Nanoimaging Spectroscopy of Semiconductor Quantum Structures in the Research Field of Nano-optics, Young Scientist's Prize, the Commendation for Science and Technology, Ministry of Education, Culture, Sports, Science and Technology, 11 April 2006.

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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 2006)

Grants

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

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

KEGG DRUG Database

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

These relationships between bio-systems and external compounds include interaction between cell and drug. At present, discovery of new drugs with desired physico-chemical and biological properties has been a long-standing challenge in pharmaceutical researches. Most of current drugs have evolved from original compounds found by chance through empirical screening. In the process of this evolution, continuous modifications have been made in an empirical manner to optimize targets to new molecules with better efficacy. It is possible to extract such a manner from a lot of data.

The KEGG DRUG database is a new addition to the KEGG LIGAND database, which contains the chemical structures of drugs and additional information such as therapeutic categories and target molecules. In particular,

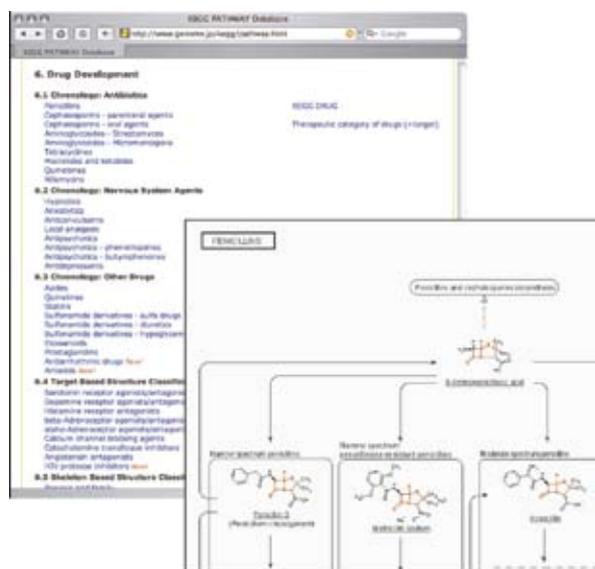


Figure 1. The KEGG DRUG Structure Map.

the KEGG DRUG Structure Map graphically illustrates our knowledge on drug development on the basis of chronology, targets and skeletons. This useful information must help new drug discovery.

GENIES: Gene Network Inference Engine Based on Supervised Analysis

The GENIES is a newly developed system to infer a global gene network consisting of functional associations between genes based on various genomic information and high-throughput experimental data (e.g., gene positions, phylogenetic profiles, gene expression profiles and protein intracellular localization) in the framework of supervised network inference. Figure 2 shows an illustration of the procedure in the GENIES. The GENIES enables us to predict unknown functional relationships between genes, and fill in the pathway holes by selecting candidate genes coding for missing enzymes in metabolic pathways.

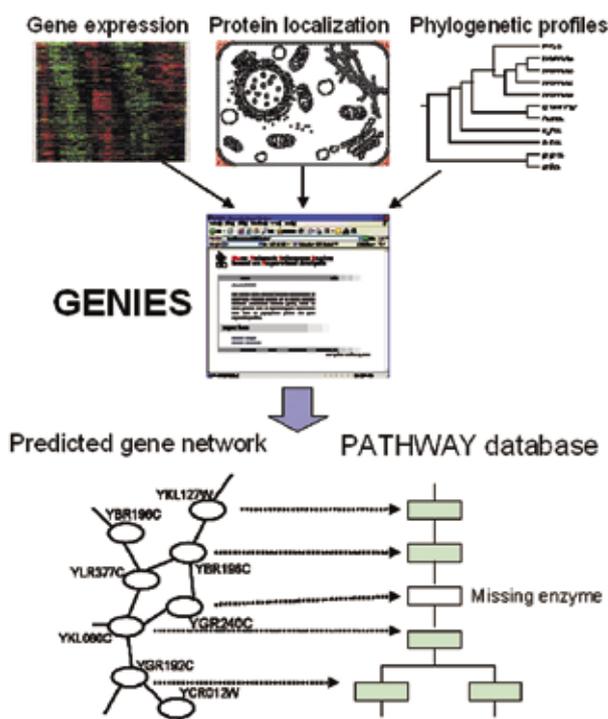


Figure 2. Various genome-wide datasets are used for predicting a global gene network.

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

Kanehisa M, Deciphering Systemic Biological Functions by Integration of Genomic and Environmental Infor-

mation, Bioinformatics Research and Development, JST.

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

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>



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Ms ZHANG, Shuqin The University of Hong Kong, China, 1 April–30 June 2006

Prof SMOLA, Alex J National Information and Communications Technology, Australia, 13 October 2006

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 2006)

Presentations

On the Complexity of Finding Control Strategies for Boolean Networks, Akutsu T, Hayashida M, Ching W-K, Ng M, The 4th Asia-Pacific Bioinformatics Conference, 15 February.

Topological Aspects of Protein Networks, Nacher JC, Hayashida M, Akutsu T, Workshop on Emergent Intelligence on Networked Agents, 8 May.

Theoretical and Computational Analyses of Structures of Metabolic Networks and Protein-protein Interaction Networks, Akutsu T, Nacher JC, The First International Conference on Computational Systems Biology, 21 July.

Multiple Methods for Protein Side Chain Packing Using Maximum Weight Cliques, Brown JB, K.C. D, Tomita E, Akutsu T, The 6th International Workshop on Bioinformatics and Systems Biology, 24 July.

Identification of Metabolic Units Induced by Environ-

mental Signals, Nacher JC, Schwartz J-M, Kanehisa M, Akutsu T, The 14th Annual International Conference on Intelligent Systems for Molecular Biology, 7 August.

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, Goto S, Mochizuki A, Tokita K, Mathematical Analysis of Structure and Dynamics of Biological Information Networks, Grant-in-Aid 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.

Identification of Metabolic Units Induced by Environmental Signal

Biological cells continually need to adapt the activity levels of metabolic functions to changes in their living environment. Although genome-wide transcriptional data have been gathered in a large variety of environmental conditions, the connections between the expression response to external changes and the induction or repression of specific metabolic functions have not been investigated at the genome scale.

We present here a correlation-based analysis for identifying the expression response of genes involved in metabolism to specific external signals, and apply it to analyze the transcriptional response of *Saccharomyces cerevisiae* to different stress conditions. We show that this approach leads to new insights about the specificity of the genomic response to given environmental changes, and allows us to identify genes that are particularly sensitive to a unique condition. We then integrate these signal-induced expression data with structural data of the yeast metabolic network and analyze the topological properties of the induced or repressed sub-networks. They reveal significant discrepancies from random networks, and in particular exhibit a high connectivity, allowing them to be mapped back to complete metabolic routes.

Nacher J.C., Schwartz J-M., Kanehisa M., Akutsu T., *Bioinformatics*, **22**, e375-e383 (2006).

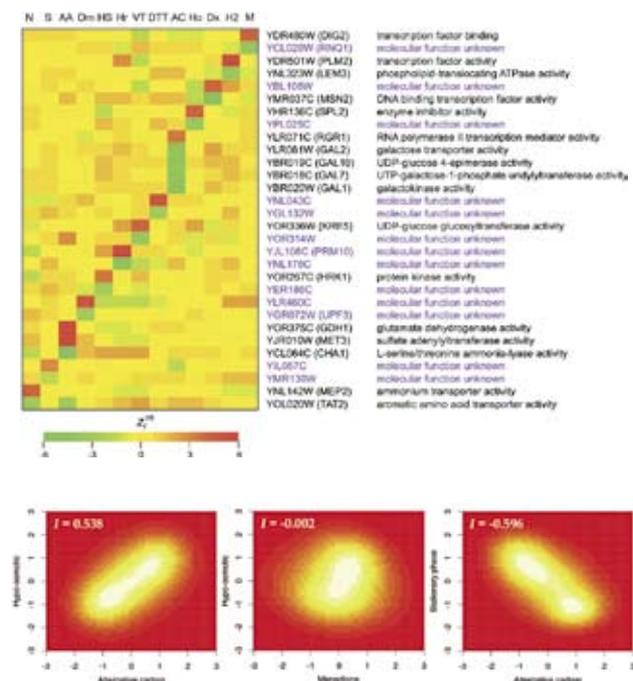


Figure 1. (Top) Genes with a unique response to specific signals. (Bottom) Representative examples of density distributions of pairs of z_i (s) scores.

A Novel Clustering Method for Analysis of Biological Networks Using Maximal Components of Graphs

Clustering is one of fundamental techniques in bioinformatics. Indeed, many clustering methods have been developed and/or applied for analyzing various kinds of biological data. However, these clustering methods such as widely used linkage methods are based on similarities between two elements or two clusters, and relations with other elements or clusters are not so much taken into account. Relations between biological entities are often represented as networks or (almost equivalently) graphs. Since such networks are considered to have much information, clustering based on network structures might be useful. The set of all maximal components of a graph essentially contains all information on minimum cuts for all pairs of nodes, where a maximal component is a set of nodes with high connectivity. It is known that a set of maximal components constitutes a laminar structure, which is essentially a hierarchical structure. Thus, we develop a novel clustering method using maximal components for an undirected network. In this method, nodes are partitioned into clusters by selecting disjoint maximal components. In this study, we apply the proposed method to clustering of protein sequences and compare with the single-linkage, complete-linkage and average-linkage methods. We evaluate the computed clusters using P -values for GO (GeneOntology) terms. The results suggest the effectiveness of the proposed method.

Hayashida M., Akutsu T., Nagamochi H., *Proc. 5th Asia-Pacific Bioinformatics Conference*, in press.

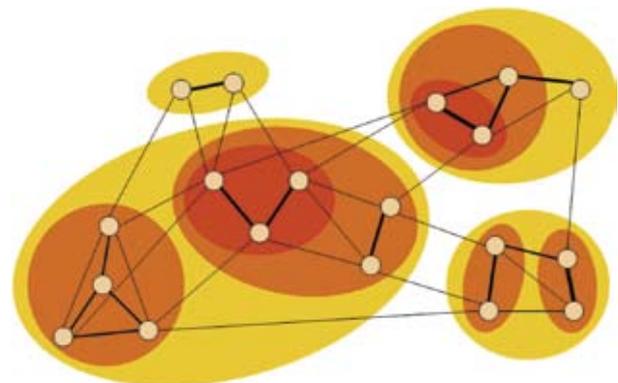


Figure 2. An example of maximal components of a graph.

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(Ph D)

Visitors

Dr ANGELOPOULOS, Nikolaos University of Edinburgh, UK, 8–29 October 2006

Prof WONG, Limsoon

National University of Singapore, Singapore, 15 December 2006

Scope of Research

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

Research Activities (Year 2006)

Presentations

Gene Sequence Ranking Based on Expression Profiles for Metabolic Pathway Analysis, SigBio Meeting, Information Processing Society of Japan, Takigawa I and Mamitsuka H, Sapporo, Japan, 9 February.

A Probabilistic Model-based Approach for Biomedical Text Mining, Mamitsuka H, First Japan-Taiwan Bilateral Symposium on Bioinformatics, Tokyo, Japan, 14 March.

ProfilePSTMM: Capturing Tree-structure Motifs in Carbohydrate Sugar Chains, Aoki-Kinoshita K F, Ueda N, Mamitsuka H and Kanehisa M, Fourteenth International Conference on Intelligent Systems for Molecular Biology (ISMB 2006), Fortaleza, Brazil, 7 August.

A New Efficient Probabilistic Model for Mining Labeled Ordered Trees, Hashimoto K, Aoki-Kinoshita K F, Ueda N, Kanehisa M and Mamitsuka H, Twelfth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2006), Philadelphia, USA, 23 August.

Applying Gaussian Distribution-dependent Criteria to Decision Trees for High-Dimensional Microarray Data, Wan R, Takigawa I and Mamitsuka H, VLDB Workshop on Data Mining in Bioinformatics, Seoul, Korea, 11 September.

Machine Learning and Pattern Recognition Using Mathematica, Takigawa I, Japan Mathematica Users Group Workshop 2006, Kobe, Japan, 28 October.

Learning Probabilistic Models for Mining Labeled Ordered Trees, Mamitsuka H, Third Japanese-German Frontiers of Sciences Symposium, Heidelberg, Germany, 3 November.

Learning a Probabilistic Model for Labeled Ordered Trees, Mamitsuka H, Second Taiwan-Japan Bilateral Symposium on Bioinformatics, Tainan, Taiwan, 9 November.

Learning a Probabilistic Model for Labeled Ordered Trees, Mamitsuka H, Workshop on Scientific Computing: Models, Algorithm and Applications, Hong Kong, China, 8 December.

Grants

Mamitsuka H, Probabilistic Model-based Method for Mining from Structured Data in Bioinformatics, Research Grant from Okawa Foundation for Information and Telecommunications, 1 September 2005–31 August 2006.

Mamitsuka H, Developing a Parameter Estimation Method for Efficient Systems Biology Based-on Machine Learning, Research Grant from Kayamori Foundation of Information Science Advancement, 1 January 2006–31 December 2007.

Takigawa I, Large-Scale Biological Information Processing Based on Computational Geometric Structures and Adaptive Sampling, Grant-in-Aid for Young Scientist (B), 1 April 2006–31 March 2008.

A New Efficient Probabilistic Model for Mining Labeled Ordered Trees

Mining frequent patterns is a general and important issue in data mining. Complex and unstructured (or semi-structured) datasets have appeared in major data mining applications, including text mining, web mining and bioinformatics. Mining patterns from these datasets is the focus of many of the current data mining approaches. We focus on labeled ordered trees, typical datasets of semi-structured data in data mining, and propose a new probabilistic model and its efficient learning scheme for mining labeled ordered trees. The proposed approach significantly improves the time and space complexity of an existing probabilistic modeling for labeled ordered trees, while maintaining its expressive power. We evaluated the performance of the proposed model, comparing it with that of the existing model, using synthetic as well as real datasets from the field of glycobiology. Experimental results showed that the proposed model drastically reduced the computation time of the competing model, keeping the predictive power and avoiding overfitting to the training data. Finally, we assessed our results using the proposed model on real data from a variety of biological viewpoints, verifying known facts in glycobiology.

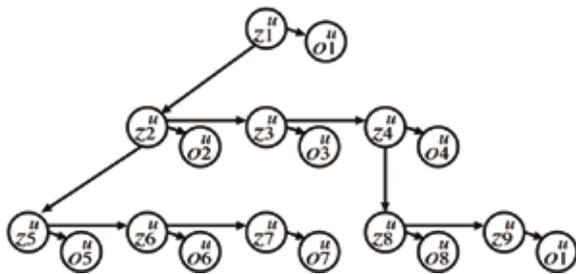


Figure 1. Graphical model of the proposed probabilistic model.

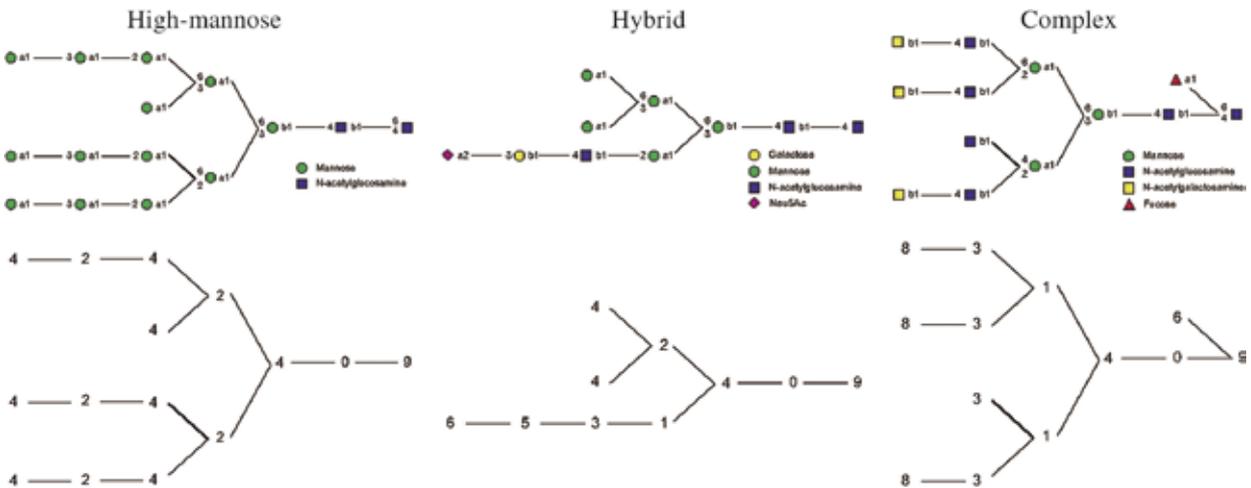


Figure 2. (top) The actual glycans, and (bottom) the most likely state paths.

Applying Gaussian Distribution-Dependent Criteria to Decision Trees for High-Dimensional Microarray Data

Biological data presents unique problems for data analysis due to its high dimensions. Microarray data is one example of such data which has received much attention in recent years. Machine learning algorithms such as support vector machines (SVM) are ideal for microarray data due to its high classification accuracies. However, sometimes the information being sought is a list of genes which best separates the classes, and not a classification rate. Decision trees are one alternative which do not perform as well as SVMs, but their output is easily understood by non-specialists. A major obstacle with applying current decision tree implementations for high-dimensional datasets is their tendency to assign the same scores for multiple attributes. We then propose two distribution-dependant criteria for decision trees to improve their use fullness for microarray classification. We empirically demonstrated the advantage of the presented distributions using a variety of real microarray datasets as well as synthetic datasets.

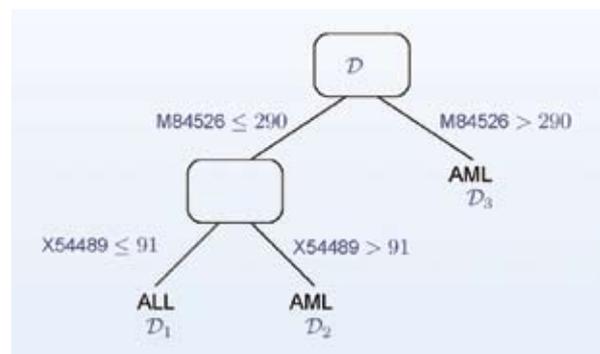


Figure 3. A typical example of a decision tree.

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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 2006)

Presentations

Evolutionary Analysis of Proteins Relevant to Quorum Sensing, Ichihara H, Kuma K, Toh H (Medical Institute of Bioregulation, Kyushu University), 20th IUBMB Int'l Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress, Japan, 21 June.

A Study of Relationship between Mammalian Specific Features and Gene Diversification on the Basis of Genome Comparisons, Kuma K, 7th Society of Evolutionary Studies, Japan, 30 August.

Positive Selection in CSP-ComD System of Streptococcal Species, Ichihara H, Kuma K, Toh H (MiB, Kyushu Univ.), MBSJ 2006 Forum, Japan, 7 December (Oral Presentation).

Relationship between Data Size and Accuracy of Prediction of Protein-Protein Interactions by Co-evolutionary Information, Sato T, Yamanishi Y, Ichihara H, Kuma K, Kanehisa M, Toh H (MiB, Kyushu Univ.), 17th Int'l Conference on Genome Informatics, Japan, 18–20 December.

Grant

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.

Partial Correlation Coefficient between Distance Matrices as a New Indicator of Protein-Protein Interactions

The computational prediction of protein-protein interactions is currently a major issue in bioinformatics. Recently, a variety of co-evolution-based methods have been investigated toward this goal. In this study, we introduced a partial correlation coefficient as a new measure for the degree of co-evolution between proteins, and proposed its use to predict protein-protein interactions.

The accuracy of the prediction by the proposed method was compared with those of the original mirror tree method and the projection method previously developed by our group. We found that the partial correlation coefficient effectively reduces the number of false positives, as compared with other methods, although the number of false negatives increased in the prediction by the partial correlation coefficient. The R script for the prediction of protein-protein interactions reported in this manuscript is available at <http://timpani.genome.ad.jp/~parco/>

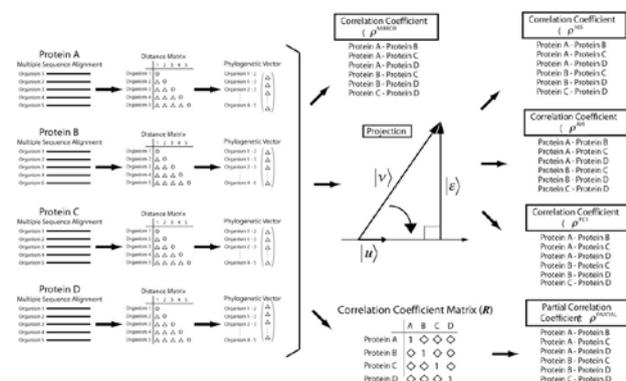


Figure 1. A schematic representation of the procedures for predicting interaction partners.

Adaptive Evolution in the ComC-ComD System of Streptococcal Species

ComC and ComD of the streptococcal species are a peptide pheromone and its receptor, respectively, which are involved in the regulation of natural DNA uptake from the environment. Both ComC and ComD show high sequence variability. Recombination is regarded as a mechanism to generate the sequence diversity. In this study, we investigated another possibility for generating sequence

diversity, adaptive point mutation, after excluding the effect of recombination as much as possible. We evaluated the rate of the number of non-synonymous substitutions per site to the number of synonymous substitutions per site by two different methods. The results of both approaches suggested that the C-terminal region of ComC and the N-terminal region of ComD have undergone positive selection. In addition, the binding specificity of ComC to the cognate ComD suggests that the adaptive change may have occurred through co-evolution between ComC and ComD. The meaning of the positive selection in the ComC-ComD system is discussed from the viewpoint of competition among the streptococcal strains for DNA resources.

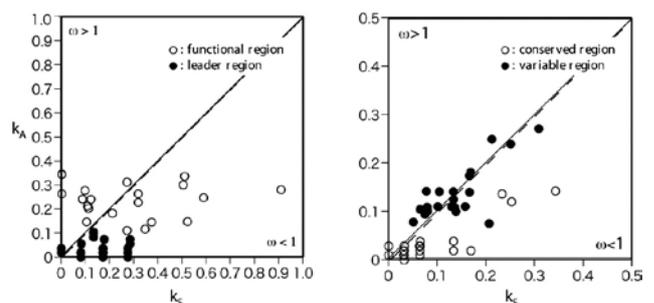


Figure 2. The k_A values are plotted as a function of the k_S values. If a plot is present above the diagonal dashed line, then the omega value for the pair corresponding to the plot is >1.0 .

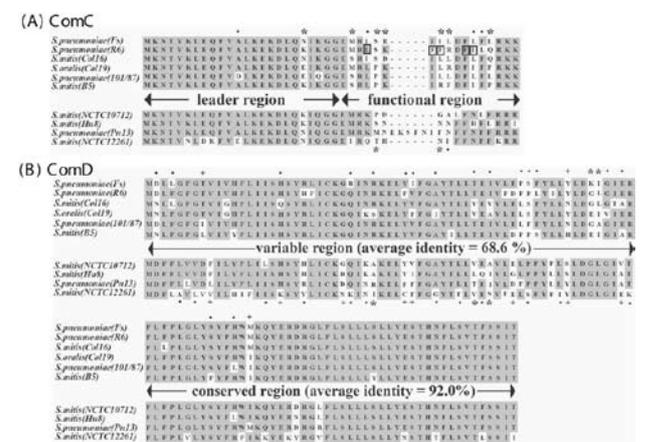


Figure 3. Multiple alignments of the ComC (A) and ComD (B) amino acid sequences. The asterisks, plus signs, and period symbols indicate the amino acid sites that correspond to the codon sites that have an omega of >1.0 , with posterior probabilities higher than 99, 95, and 50%, respectively.



VISITING PROFESSORS'
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Lecture at ICR

Interfacial Interactions between Synthetic Polymers and Proteins



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Lecture at ICR

Behavior of Trace Chemical Components in Hydrothermal Plume –Methane and Rare Earth
Elements in the Okinawa Trough– (2 March 2007)



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Lecture at ICR

Spin-polarized Electron Source



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Lecture at ICR

Genomic Drug Discovery



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Lectures at ICR

Complex Oxide Heteroepitaxy
Correlated Electrons at Interfaces and in Confined Systems



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Lecture at ICR

Arginine in Protein Research: Mechanisms and Application to Solubilization and Chromatography



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Laboratory of Molecular Aggregation Analysis
Associate Professor, The Institute for Solid State Physics, The University of Tokyo
(5-1-5, Kashiwanoha, Kashiwa 277-8581)

Lecture at ICR

Biomaterials-Based Light Emitting Diodes – BIODIODE



Vis Assoc Prof
YAMADA, Yoichi
(D Eng)

Laboratory of Photonic Elements Science
Associate Professor, Department of Electrical and Electronic Engineering, Yamaguchi University
(Tokiwadai, Ube, Yamaguchi 775-8611)

Lecture at ICR

Localized Biexciton States in AlGaIn Semiconductor Alloy



Vis Assoc Prof
DEMÉ, Bruno
(Ph D)

Laboratory of Molecular Rheology
Chief Beam Line Scientist, Institute Laue-Langevin
(6, rue Jules Horowitz, BP 156-38042 Grenoble Cedex 9, France)

Lecture at ICR

New Shapes in Surfactant and Lipid Self-Assembly



Vis Assoc Prof
LEONG, Weng Kee
(Ph D)

Laboratory of Organotransition Metal Chemistry
Associate Professor, Department of Chemistry, Faculty of Science, National University of Singapore
(Block 59, #05-05, Kent Ridge Crescent, Singapore 119260)

Lecture at ICR

Our Attempts at Connecting Organometallic Clusters with Nanoscience and Biology

A decorative graphic consisting of two horizontal lines and two vertical lines. The top horizontal line starts from the left edge and ends with a small dark square. The bottom horizontal line starts from the left edge and ends with a small dark square. A vertical line on the left side connects the top and bottom horizontal lines. Another vertical line on the right side connects the top and bottom horizontal lines.

PERSONAL

Retirement

Professor FUKUDA, Takeshi
Division of Materials Chemistry
— Chemistry of Polymer Materials —



On March 31st, 2007, Dr. Takeshi Fukuda retired from Kyoto University after 34 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Fukuda was born in Kyoto on October 28th, 1943. He graduated from Department of Polymer Chemistry, Faculty of Engineering, Kyoto University in 1967 and subsequently entered Graduate School of Engineering, Kyoto University, where he took the master and then doctoral programs, studying solution properties of copolymers under the supervision of the late Professor Hiroshi Inagaki. In 1973, he was granted a doctoral degree with a thesis entitled “Some Behavior of Block Copolymer Chains in Solution”. In 1972, he had a position of research associate at Institute for Chemical Research, Kyoto University (ICR) and was appointed Assistant Professor (1977), Associate Professor (1990), and Full Professor (2001) at ICR, directing the Laboratory of Design of Polymer Materials at that time.

Throughout his academic carrier, Dr. Fukuda has devoted himself to studies on both synthesis and properties of polymers and polymer materials on the basis of physicochemical approaches.

His achievements in the field of polymer properties include his invention of the light scattering method known as the “optical theta-solvent method”, which permitted selective observation and precise analysis of the interactions between unlike polymers and the compositional heterogeneity of copolymers, and his establishment of the theoretical model relevant to “orientation-dependent excluded-volume effect”, which was useful for a systematic understanding of orientation-dependent phenomena such as the nematic-isotropic phase transition in semi-flexible polymers and the induced segmental orientation and orientation-induced phase separation in polymer blends.

In the field of polymer synthesis, he was the first to experimentally determine the propagation and termination rate constants in free radical copolymerization. By a series of precise experiments, he disclosed the general failure of the Mayo-Lewis copolymerization model with respect to absolute rate constants, showing that the penultimate-unit effect was responsible for the failure of the classic model. He also established a new velocity equation of copolymerization by experimentally proving that the termination step in copolymerization was not chemically controlled, as had been so believed for a long time, but diffusion controlled.

More recently, Dr. Fukuda has made pioneering contributions to the establishment of the kinetic theory of living radical polymerization (LRP), which has rapidly developed for this decade or so, as a new versatile and robust method of precise synthesis of polymers. At the same time, he has applied LRP to the synthesis of a variety of new polymers and polymer materials. In particular, he and his co-workers were the first to establish the technique of surface-initiated LRP on various substrates to produce polymer-grafted surfaces with ultra-high graft density or “concentrated polymer brushes”.

These achievements of Dr. Fukuda have been published as over 250 scientific publications including original papers, reviews, and book chapters and are highly appreciated internationally as well as in Japan. He was granted the Award of the Society of Polymer Science, Japan (1992) for the work on copolymerization kinetics and the Grant-in-Aid for Specially Promoted Research (2005–2008) for the work on concentrated polymer brushes and LRP.

His contribution to ICR and Kyoto University through his scientific and educational activities is hereby gratefully acknowledged.

Retirement

Professor SAKATA, Kanzo

Division of Biochemistry

— Chemistry of Molecular Biocatalysts —



On March 31st, 2007, Dr. Kanzo Sakata retired from Kyoto University after 9 years of service and was honored with the title of Professor Emeritus of Kyoto University. Dr. Sakata was born in Shiga Prefecture on August 6th, 1943. He graduated from Department of Agricultural Chemistry, Faculty of Agriculture, Kyoto University in 1966. He started his research career on natural product chemistry in Graduate School of Agriculture, Kyoto University under the supervision of late Professor T. Mitsui. After completing his Master's degree in 1968, he proceeded to the doctoral program. During the doctoral study, in 1970, he was appointed as a Researcher of the Institute of Physical and Chemical Research (RIKEN). He continued his study and was granted a doctoral degree for a thesis entitled "Studies on a Piscicidal Constituent of *Hura crepitans*" in 1972. On leave from RIKEN, from 1977 to 1979, he studied the chemistry of bioactive isocyanates under Dr. R. Rickard at Research School of Chemistry, Australian National University in Canberra as a Research Fellow. In 1981, he was appointed as an Associate Professor of Department of Agricultural Chemistry, Faculty of Agriculture, Shizuoka University and was promoted to a Professor of the university, Laboratory of Marine Biological Science, in 1987. He was transferred to Institute for Chemical Research, Kyoto University in 1998.

Dr. Sakata devoted himself mainly to the chemistry of biologically active natural products such as an active principle of a piscicidal plant, antibiotics for agricultural use, feeding stimulants for marine gastropods, settlement retardants for marine fouling organisms, *etc.* He was awarded a prize for young active scientists from Japan Society of Agricultural Chemistry for the study on the chemical studies of Ezomycins for agricultural use in 1975.

He also extended his interests to studies on tea from new viewpoints since he moved to Shizuoka University. Being interested in the beautiful floral aroma of oolong tea, he tried to elucidate the molecular basis of the floral aroma formation during the oolong tea manufacturing by applying research technologies in natural product chem-

istry, biochemistry, and molecular biology. The results of his studies showed that the floral tea aroma is produced as the results of self-defense mechanism responding to various kinds of stresses applied on leaves of tea plants during the manufacturing processes. Furthermore he studied the molecular basis of the profound aroma formation of the famous Formosa oolong tea, Oriental Beauty, and the Darjeeling Second Flash, that are produced from tea leaves infested by particular species of insects, he showed that the insect infestation is very important for each tea to have the characteristic tea aroma. Based on the knowledge he obtained through these studies, he is trying to improve the quality of black tea or to make new type of black tea by collaborating with scientists of Tea Research Association, India. His contribution to development of tea science was appreciated and he was awarded 34th Tocklai Conference Award by TRA India in 2005.

When he was appointed as a Professor of Kyoto University, he decided to organize a team comprising of young staff members with diversified research backgrounds including a natural product chemist, an organic synthetic chemist, and a plant molecular biologist. The team can nurture students who can well understand organic chemistry and apply molecular biological methods when need. His young collaborators have developed wide range of research projects that can be done by such a unique research group; its successful achievements include identification of cytochrome P450 genes involved in a new route of biosynthesis/metabolism of plant hormones such as brassinosteroids and abscisic acid, a challenging approach to clarify the key enzymes in homeostasis in auxins as well as a key enzyme in coumarin biosynthesis.

All the achievements, which are results of the contribution with his dedicated colleagues and students, have been published as 148 original articles in international journals and 91 accounts, reviews and books. His contribution to Kyoto University through his scientific and educational activities is hereby gratefully acknowledged.

Retirement

Professor TAKANO, Mikio

International Research Center for Elements Science

— Advanced Solid State Chemistry —



On March 31st, 2007, Dr. Mikio Takano retired from Kyoto University after 25 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Takano was born in Kyoto on March 7th, 1944. He graduated from Department of Chemistry, Kyoto University in 1966. He studied the magnetic properties of various compounds containing iron with Mössbauer spectroscopy at the Graduate School of Science under supervision of Prof. Toshio Takada, and was granted a doctoral degree in 1973.

In 1972 he was appointed as a research associate of Department of Chemistry, Konan University. In 1983 he moved to the Institute for Chemical Research, Kyoto University, and he was promoted to a full professor in 1993 directing the Laboratory of Solid State Chemistry (presently re-named as Advanced Solid State Chemistry). During 2002–2005, he served as the director of the institute and faced the historical change of Kyoto University from a national university to a “national university corporation”. On an educational ground, he has given a regular course on Solid State Chemistry at the Graduate School of Science, Kyoto University and supervised the dissertation works of graduate students.

During his academic carrier, Dr. Takano devoted himself to solid state chemistry (SSC) of 3d transition metal oxides and made a number of notable findings. The discovery of the charge disproportionation of Fe^{4+} ion into Fe^{3+} and Fe^{5+} in CaFeO_3 (1977) attracted considerable attention in the fields of solid state chemistry and physics, and he was invited as an associate prof. of Bordeaux University I which was one of the three biggest world SSC centers. Dr. Takano was actively involved in the worldwide “High- T_c fever” produced by the discovery of high- T_c superconductivity in cupric oxides (1986). He found an efficient formation process of a superconductor called the Bi-2223 phase, which triggered off the development of industrial potential as a superconducting power cable, for example. Since this time, however, he and his colleagues

began to search for genuinely new, chemically and physically interesting oxides using a high pressure technique. New superconductors such as $(\text{Ca},\text{Na})_2\text{CuO}_2\text{Cl}_2$ and also antiferromagnetic quantum spin ladders like SrCu_2O_3 and $\text{Sr}_2\text{Cu}_3\text{O}_5$ which represent the very initial stage of dimensional crossover from 1D to 2D were thus discovered. More recently his group has extended their preparative techniques to obtain films and nano-sized particles.

He authored and co-authored more than 400 research articles and letters, including those published in the most important international journals such as *Nature*, *Nature Materials*, and *Science*. For these distinguished contributions, he was invited as an invited prof. of Grenoble Univ. I (1998) and of Bordeaux Univ. I (1977, 1999). He was presented the JSPM Award for Innovatory Research in 1980 and 1994, and Award for Distinguished Achievements in Research in 2002 (JSPM: Japan Society of Powder and Powder Metallurgy), Award of Merit '97 from The Society of Non-Traditional Technology – New Superconducting Materials Forum, and The L’Oreal Art & Science of Color Prizes: The 8th Gold Prize in 2005. He also made a great effort to develop the SSC in Japan by taking an initiative to hold the first international conference on SSC in Japan.

Dr. Takano also contributed to various scientific societies. He has been an editor and a member of the editorial board of international journals including *Solid State Sciences*, *Journal of Solid State Chemistry*, and others. He has been a vice president of JSPM and an advisor of Japan Science and Technology Agency. He has tried to promote collaborations with industries also: He has served as an auditor of a company which has produced iron oxides for almost 200 years.

His contribution to Kyoto University through his scientific, educational and administrative activities is gratefully acknowledged. His sincere and warmhearted personality has been admired by his friends, colleagues, and especially by his students.

Awards

SASAMORI, Takahiro



ICR Award for Young Scientists

“Double-bond Compounds between Heavier Group 15 Elements”

Institute for Chemical Research

15 December 2006

MIZUHATA, Yoshiyuki



The Student Lecture Award

The 86th Annual Meeting of the Chemical Society of Japan

“Synthesis, Isolation, and Properties of the First Stable Neutral Stannaromatic Compounds”

The Chemical Society of Japan

May 2006

NAGAHORA, Noriyoshi



The Best Oral Presentation Award

The 86th Annual Meeting of the Chemical Society of Japan

“Syntheses, Structures, and Properties of Kinetically Stabilized 1,1'-Bis(diphosphenyl)ferrocenes”

The Chemical Society of Japan

May 2006

MURATA, Yasujiro



Osawa Award

The 30th Fullerene Nanotubes General Symposium

“Reactions and Electrochemical Properties of Endohedral Fullerene, $H_2@C_{60}$ ”

The Fullerenes and Nanotubes Research Society

8 January 2006

Young Scientists' Prize, The Commendation for Science and Technology

“Structural Transformation of Fullerenes in the Field of Nano-carbon”

MEXT

18 April 2006

MURATA, Michihisa



President Prize of Kyoto University

“Studies on Organo-Chemical Transformations of Fullerenes”

Kyoto University

20 March 2006

OHNO, Kohji



The Award for Encouragement of Research in Polymer Science

“Precision Design of Organic/Inorganic Hybrid Materials by Living Radical Polymerization”

The Society of Polymer Science, Japan

25 May 2006

KASAI, Shinya



ICR Award for Young Scientists

“Current-Driven Resonant Excitation of Magnetic Vortices”

Institute for Chemical Research

15 December 2006

MIZUTANI, Masaharu



The JSCR Award for the Encouragement of Young Scientists

“Biochemical Studies on Cytochrome P450 Monooxygenases in Abscisic Acid and Plant Steroid Metabolism”

The Japanese Society for Chemical Regulation of Plants

30 October 2006

HIMENO, Atsushi



ICR Award for Graduate Students

“Domain Wall Ratchet Effect Induced by an Electric Current”

Institute for Chemical Research

15 December 2006

TSUGE, Tomohiko



Awarded Guest Professor of Brain Korea 21 Silver-Bio Research Center

“COP9 Signalosome: The Key Modulator of Signal Transduction in Plants and Mammals”

Dong-A University, Busan, KOREA

1 March 2006–28 February 2007

NAKASE, Ikuhiko



The Best Presentation Award

The First FIP-APSTJ Joint Workshop on Gene Delivery, Sapporo

“Selective Modification of N-glycosides of Transferrin with Therapeutic Drugs for the Receptor Targeting”

International Pharmaceutical Federation and Academy of Pharmaceutical Science and Technology, Japan

24 July 2006

UESUGI, Motonari



Tokyo Techno-Forum 21 Gold Medal Award

“Small-molecule Based Chemical Genetic Research for Biological Investigation”

12 April 2006

MATUBAYASI, Nobuyuki



Young Scientists' Prize, The Commendation for Science and Technology

“Study of the Structure and Reactions of Supercritical Water in the Field of Physical Chemistry”

MEXT

18 April 2006

HATAKEYAMA, Takuji



Kaneka Award in Synthetic Organic Chemistry

“Development of SN_2 Reaction of Carbon–Heteroatom Bond with Highly Reactive Metal Enolate”

The Society of Synthetic Organic Chemistry, Japan

30 November 2006

FADIL, Hicham



PASJ Award for Young Scientists

“Proof of Electron Cooling of Hot Ion Beams, Particle Accelerator Society of Japan”

Particle Accelerator Society of Japan

4 August 2006

YAMAMOTO, Shinpei



MSJ Outstanding Presentation Award

The 30th Annual Conference on Magnetism in Japan

“Preparation of $L1_0$ -FePt Nanoparticles Dispersible in Nonpolar Organic Solvents”

The Magnetism Society of Japan

22 November 2006

NAKAMURA, Masaharu



Lectureship Award to China

1st International Conference on Cutting-Edge Organic Chemistry in Asia

“Iron-Catalyzed Cross-Coupling of Haloalkanes”

JSPS Asian CORE Program Project Committee

20 October 2006

Lectureship Award to Hong-Kong

1st International Conference on Cutting-Edge Organic Chemistry in Asia

“Iron-Catalyzed Cross-Coupling of Haloalkanes”

JSPS Asian CORE Program Project Committee

20 October 2006

Banyu Young Chemist Award 2006

“Development of Some New C–C Bond Forming Reactions toward Exploitation of Chemical Resources”

Banyu Life Science Foundation International

18 November 2006

KANEMITSU, Yoshihiko



Inoue Prize for Science

“Pioneering and Outstanding Contributions to Nano-silicon Optoscience”

Inoue Foundation for Science

3 February 2006

Yazaki Memorial Foundation Award

“Outstanding Contributions to Semiconductor Nanoparticle Optoscience”

Yazaki Foundation

9 March 2006

MATSUDA, Kazunari



Young Scientist's Prize, The Commendation for Science and Technology

“Nanoimaging Spectroscopy of Semiconductor Quantum Structures in the Research Field of Nano-optics”

MEXT

18 April 2006

Paper Awards

NAKAMURA, Kaoru



Tetrahedron: Asymmetry Most Cited Paper 2003–2006 Award

“Recent Developments in Asymmetric Reduction of Ketones with Biocatalysts”

Elsevier Limited

October 2006

KAWABATA, Takeo



Tetrahedron Letters Most Cited Paper 2003–2006 Award

“Preparation and Properties of Chiral 4-Pyrrolidino-pyridine (PPY) Analogues with Dual Functional Side Chains”

Elsevier Limited

10 September 2006

Poster Awards

MATSUMOTO, Teruyuki



The Best Poster Award

18th Symposium on Fundamental Organic Chemistry

“Synthesis of the First β -Ketophosphenato Ligand by Taking Advantage of Steric Protection and Its Structure”

The Chemical Society of Japan and the Kinki Chemical Society, Japan

9 October 2006

MORIYAMA, Katsuhiko



Best Poster Award

The 23rd Seminar on Synthetic Organic Chemistry (Sapporo)

“Asymmetric Cyclization of Amino Acid Derivatives with Metal Hydroxides at Room Temperature”

The Society of Synthetic Organic Chemistry, Japan

14 September 2006

SUE, Daisuke



Best Poster Award

21st Regular Meeting of Cyclophane Chemistry

“Determination of Axial Chiralities and Optical Properties of the Helical Oligonaphthalenes”

The Society of Functional Host-Guest Chemistry, Japan

1 December 2006

YOSHIKAWA, Chiaki



IUPAC Poster Prize

IUPAC Sponsored International Symposium on Radical Polymerization: Kinetics and Mechanism

“Protein Repellency of Concentrated Polymer Brushes Prepared by Surface-Initiated Living Radical Polymerization”

International Union of Pure and Applied Chemistry

9 September 2006

OHNISHI, Toshiyuki



Best Poster Award

8th International Symposium on Cytochrome P450 Biodiversity and Biotechnology, University of Wales Swansea, Swansea, Wales, UK

“Functional Characterization of Arabidopsis CYP90C1 and CYP90D1 Encoding Brassinosteroids C-23 hydroxylases”

27 July 2006

Best Poster Award

The 41st Annual Meeting of the Japanese Society for Chemical Regulation of Plants at Osaka Prefecture University, Japan

“Biochemical Characterization of Brassinosteroid C-3 Oxidase”

The Japanese Society for Chemical Regulation of Plants

30 October 2006

HIMENO, Atsushi



Best Poster Award

The 17th International Conference on Magnetism (ICM)

“Magnetic Ratchet Effect in Submicron Magnetic Wires with Asymmetric Notches”

25 August 2006

KAWAMOTO, Jun



The Best Poster Presentation Award

The 7th Annual Meeting of the Japanese Society for Extremophiles

“Functional Analysis of a Cold-Inducible Porin Involved in Cold-Adaptation of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10”

The Japanese Society for Extremophiles

28 November 2006

Obituary

Professor Emeritus

Dr. INAGAKI, Hiroshi (1924–2007)



Dr. Hiroshi Inagaki, Professor Emeritus of Kyoto University, passed away on January 20, 2007, in Kyoto.

Dr. Inagaki was born in Nagoya on December 3, 1924. He graduated from the Department of Fiber Chemistry at the Faculty of Engineering, Kyoto University, in 1946. After 6 years of research and teaching service at the same Faculty as Full-Time Lecturer, he was promoted to Associate Professor in 1954 to join Institute for Chemical Research (ICR), Kyoto University. In 1960, he was appointed Full Professor at ICR, a position that he held until retirement, to take charge of a new laboratory, the Laboratory of Polymer Properties. In accordance with the development of his research work, his laboratory was later renamed the Laboratory of Polymer Separation and Characterization. He retired from Kyoto University in 1988 and subsequently was honored with the title of Professor Emeritus of Kyoto University.

He conducted extensive research in physicochemical fields of polymer science. Specifically, his research fields included the separation and characterization of macromolecules by various means such as ultra-centrifugation, light scattering, and thin-layer and gel permeation chromatography, the structural and functionalizing studies of naturally occurring polymers such as wool and cellulose, and the properties and formation mechanisms of block, graft, and statistical copolymers. His pioneering achievements in each field are highly appreciated internationally as well as domestically. Perhaps the achievement the most widely appreciated and the most beloved by himself is related to thin-layer chromatography. He introduced this simple and non-costly technique to the polymer field, showing its versatility to characterize polymers and copolymers: for example, he showed that it enabled separation of copolymers according to composition only without the interference of chain length effect. Similar information was and is, even today, hardly obtainable by other techniques.

He gave lectures on physical chemistry of macromolecules at the Graduate School of Engineering, Kyoto University as well as at many other foreign and domestic institutions, and supervised the dissertation studies of a number of graduate students. After his retirement from Kyoto University, he continued his educational work at Mukogawa Women's University from 1989 to 1996 as professor/dean at the Graduate School.

Dr. Inagaki has also made no small contributions to the management and administration of ICR, Kyoto University, and other scientific and international communities. For example, he was director of ICR and member of the University Council, Kyoto University, for two years from April, 1984. He was president of the Society of Fiber Science and Technology, Japan (SFST), and served as chair of the Polymer Characterization Committee of the Society of Polymer Science, Japan (SPSJ) as well as several international conferences. He was much concerned about problems related to academic interaction and exchange of students and scientists with foreign countries, serving as member and chair of the International Committee, Kyoto University. Most notably, he was one of the two cofounders of "Haus der Begegnung Kyoto" (Kyoto International Student House) and had been chair of the board of trustees of the House until his death.

His sincere and warm personality was respected by many friends, colleagues, students, and all those who came in contact with him. For his distinguished scientific, educational, international, and other achievements, he was honored with the SFST Award for Outstanding Achievement and the SPSJ Award for Outstanding Achievement in Polymer Science. In 2002, the Government made public recognition of his achievements by the Second Class of the Order of the Sacred Treasure, "Kun-Ni-Tou Zuihoushou" Medal.



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

THESES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

- Kawai Y, Hayashi M, Tokitoh N: Chlorodinitrophenylhydrazine, a Useful Crystalline Agent for Absolute Configuration Determination of Various Chiral Ketones, *Tetrahedron*, **61**, 5049-5055 (2005).
- Yasui S, Itoh K, Ohno A, Tokitoh N: Dramatic Effect of N-Substituents in Viologens on Single Electron Transfer from Tributylphosphine, *Org. Biomol. Chem.*, **3**, 4188-4192 (2005).
- Shimizu D, Takeda N, Tokitoh N: Unusual Carbon-Sulfur Bond Cleavage in the Reaction of a New Type of Bulky Hexathioether with a Zerovalent Palladium Complex, *Chem. Commun.*, **2006**, 177-179 (2006).
- Shimizu D, Takeda N, Sasamori T, Tokitoh N: Bis[2-(phenylsulfanyl)benzenethiolato]palladium(II), *Acta Cryst. E*, **61**, m166-m167 (2006).
- Tajima T, Sasamori T, Takeda N, Tokitoh N, Yoshida K, Nakahara M: Synthesis of Bis(germacyclopropa)benzenes and Structures of Their Annelated Benzene Rings, *Organometallics*, **25**, 230-235 (2006).
- Sugiyama Y, Sasamori T, Hosoi Y, Furukawa Y, Takagi N, Nagase S, Tokitoh N: Synthesis and Properties of a New Kinetically Stabilized Digermene: New Insights for a Germanium Analogue of an Alkyne, *J. Am. Chem. Soc.*, **128**, 1023-1031 (2006).
- Nagahora N, Sasamori T, Tokitoh N: Syntheses, Structures, and Properties of the First Stable 1,1'-Bis(diphosphenyl)ferrocenes, *Chem. Lett.*, **35**, 220-221 (2006).
- Mizuhata Y, Sasamori T, Takeda N, Tokitoh N: A Stable Neutral Stannaromatic Compound: Synthesis, Structure and Complexation of a Kinetically Stabilized 2-Stannaphthalene, *J. Am. Chem. Soc.*, **128**, 1050-1051 (2006).
- Hiratsuka H, Horiuchi H, Furukawa Y, Watanabe H, Ishihara A, Okutsu T, Tobita S, Yoshinaga T, Shinohara A, Tokitoh N, Oba M, Nishiyama K: Photophysical and Photochemical Processes of 9,10-Dihydro-9-silaphenanthrene Derivatives: Photochemical Formation and Electronic Structure of 9-Silaphenanthrenes, *J. Phys. Chem. A*, **110**, 3868-3874 (2006).
- Hamaki H, Takeda N, Tokitoh N: Reduction of Tetravalent Group 4 Metal Complexes Supported by an Extremely Bulky, Unsymmetrically Substituted β -Diketiminato Ligand Leading to the Regioselective C=N Bond Cleavage Giving Ring-Contracted Metal-Imido Complexes, *Organometallics*, **25**, 2457-2464 (2006).
- Sasamori T, Tokitoh N: Sila- and Germacyclopropabenzenes, *Organometallics*, **25**, 3522-3532 (2006).
- Sasamori T, Inamura K, Hoshino W, Nakata N, Mizuhata Y, Watanabe Y, Furukawa Y, Tokitoh N: Synthesis and Characterization of Two Isomers of 14 π -electron Germaaromatics: Kinetically Stabilized 9-Germaanthracene and 9-Germaphenanthrene, *Organometallics*, **25**, 3533-3536 (2006).
- Tajima T, Takeda N, Sasamori T, Tokitoh N: A Kinetically Stabilized Stannanetellone, a Tin-Tellurium Double-Bond Compound, *Organometallics*, **25**, 3552-3553 (2006).
- Sasamori T, Mieda E, Nagahora N, Sato K, Shiomi D, Takui T, Hosoi Y, Furukawa Y, Takagi N, Nagase S, Tokitoh N: One-electron Reduction of Kinetically Stabilized Dipnictenes: Synthesis of Dipnictene Anion Radicals, *J. Am. Chem. Soc.*, **128**, 12582-12588 (2006).
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- Tsubaki K, Tanaka H, Takaishi K, Miura M, Morikawa H, Furuta T, Tanaka K, Fuji K, Sasamori T, Tokitoh N, Kawabata T: Bottom-Up Synthesis of Optically Active Oligonaphthalenes: Three Different Pathways for Controlling Axial Chirality, *J. Org. Chem.*, **71**, 6579-6587 (2006).
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- Nakamura K, Matsuda T: Biocatalytic Reduction of Carbonyl Group, *Current Organic Chemistry*, **10**, 1217-1246 (2006).
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- Fujii M, Fukumura M, Hori Y, Hirai Y, Akita H, Nakamura K, Toriizuka K, Ida Y: Chemoenzymatic Synthesis of Optically Active γ -alkyl- γ -butenolides, *Tetrahedron: Asymm.*, **17**, 2292-2298 (2006).

— Structural Organic Chemistry —

Nakamura T, Araki Y, Ito O, Murata Y, Komatsu K: Photoinduced Charge Separation and Charge Recombination in Terthiophene-Acetylene-Fullerene Linked Dyads, *J. Photochem. Photobiol. A*, **178**, 242-250 (2006).

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Yamazaki D, Nishinaga T, Tanino N, Komatsu K: Erthiophene Radical Cations End-Capped by Bicyclo[2.2.2]octene Units: Formation of Bent π -Dimers Mutually Attracted at the Central Position, *J. Am. Chem. Soc.*, **128**, 14470-14471 (2006).

Sartori E, Ruzzi M, Turro N J, Decatur J D, Doetschman D C, Lawler R G, Buchachenko A L, Murata Y, Komatsu K: Nuclear Relaxation of H₂ and H₂@C₆₀ in Organic Solvents, *J. Am. Chem. Soc.*, **128**, 14752-14753 (2006).

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Laboratory of Polymer Chemistry, Eindhoven University of
Technology

[Poland]

Institute of Radiation Chemistry, Department of Chemistry, Technical University of Lodz

[Russia]

Joint Institute for Nuclear Research

[South Africa]

Department of Chemistry and Polymer Science, University of Stellenbosch

[Sweden]

Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences

[Switzerland]

Department of Organic Chemistry, University of Geneva

Laboratory for Neutron Scattering, ETH Zurich and PSI Villigen

[Taiwan]

Department of Chemical Engineering, National Cheng Kung University

[UK]

Department of Physics, University of Wales Swansea

School of Chemistry, Southampton University

Welsh School of Pharmacy, Redwood Building, Cardiff University

[USA]

Ames Laboratory and Department of Physics and Astronomy, Iowa State University

Argonne National Laboratory

Cancer Genomics Core Laboratory, Department of Pathology, The University of Texas M.D. Anderson Cancer Center

Departments of Biology and Chemical and Biomolecular Engineering, The Johns Hopkins University, Baltimore, Maryland

Department of Chemical Engineering, University of California, Berkeley

Department of Chemistry, Carnegie Mellon University

Department of Chemistry, Columbia University

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

Department of Chemistry and Biochemistry, University of Southern Mississippi

Department of Physics, University of Illinois at Chicago

Department of Physics, Yale University

Howard Hughes Medical Institute and Department of Cellular and Molecular Pharmacology, University of California, San Francisco

Laboratory of Plant Molecular Biology, Rockefeller University

Materials Sciences Division, Argonne National Laboratory

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

NSF's International Materials Institute for New Functionality in Glass, Department of Materials Science and Engineering, Lehigh University

Othmer Department of Chemical & Biological Sciences & Engineering, Polytechnic University

The Verna and Marrs Mclean Department of Biochemistry and Molecular Biology, Baylor College of Medicine

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

THESES

FUKAGAWA, Daiji
D Inf, Kyoto University
“Discrete Algorithms for Optimization Problems for Structured Data in Bioinformatics”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2006

HAN, Li-You
D Agr, Kyoto University
“Studies on γ -Glutamyl Transpeptidases by Using Mechanism-Based Inhibitors”
Supervisor: Prof SAKATA, Kanzo
24 November 2006

HIZUKURI, Yoshiyuki
D Sc, Kyoto University
“Comparative Glycome Analysis and Motif Extraction”
Supervisor: Prof KANEHISA, Minoru
23 March 2006

IMAI, Kumiko
D Sc, Kyoto University
“Functional Analysis of an Arabidopsis Cyclin, AtCYCA2;3”
Supervisor: Prof OKA, Atsuhiko
23 March 2006

KAN, Daisuke
D Sc, Kyoto University
“Blue-luminescence from Off-Stoichiometric SrTiO₃ and Fabrication of the Device Structure”
Supervisor: Prof TAKANO, Mikio
23 March 2006

K.C., Dukka Bahadur
D Inf, Kyoto University
“Clique-based Algorithms for Protein Structure Prediction”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2006

KITAGAWA (ISHIDA), Norihiro
D Sc, Kyoto University
“Functional Analysis of the Transcription Factor NFAT2 during Osteoclastogenesis”
Supervisor: Prof OKA, Atsuhiko
23 March 2006

KONISHI, Takashi
D Eng, Kyoto University
“Polymer Crystallization through Intermediate State”
Supervisor: Prof KANAYA, Toshiji
23 March 2006

KUNIYOSHI, Minoru
D Eng, Kyoto University
“Studies on Phenyl-modified Polysiloxane Low-melting Glass: Preparation through Sol Concentration Method and Rapid Heat Treatment”
Supervisor: Prof YOKO, Toshinobu
24 November 2006

KWAK, Yungwan
D Eng, Kyoto University
“Kinetic Studies on Living Radical Polymerizations”
Supervisor: Prof FUKUDA, Takeshi
23 March 2006

MINARI, Takeo
D Sc, Kyoto University
“Fabrication and Characterization of Organic Field-Effect Transistor”
Supervisor: Prof ISODA, Seiji
23 March 2006

MIYATA, Yasuo
D Eng, Kyoto University
“Studies on Synthesis and Properties of π -Conjugated Systems Directed to Organic Field-Effect Transistor”
Supervisor: Prof KOMATSU, Koichi
23 March 2006

MIZUHATA, Yoshiyuki
D Sc, Kyoto University
“Syntheses and Properties of Kinetically Stabilized Tin-carbon Double-bond Compounds”
Supervisor: Prof TOKITOH, Norihiro
23 March 2006

MIZUNO, Megumi
D Eng, Kyoto University
“Study on Novel Organic-inorganic Hybrid Low-melting Glass: Preparation through Nonaqueous Acid-Base Reaction and Application as Photonic Materials”
Supervisor: Prof YOKO, Toshinobu
23 March 2006

MURATA, Michihisa
D Eng, Kyoto University
“Organic Synthesis of Endohedral Fullerenes Encapsulating Molecular Hydrogen”
Supervisor: Prof KOMATSU, Koichi
23 March 2006

NAGAO, Masato
D Eng, Kyoto University
“Studies of Transition-Metal-Catalyzed Reactions for Precise Control of Primary Structures of Functional Polymers”
Supervisor: Prof OZAWA, Fumiyouki
23 March 2006

NAKAO, Mitsuteru
D Sc, Kyoto University
“Large-scale Analysis of Human Alternative Protein Isoforms: Pattern Classification and Correlation with Subcellular Localization Signals”
Supervisor: Prof KANEHISA, Minoru
23 March 2006

NAKAO, Toshio
D Eng, Kyoto University
“Formulation and Application of Analytical Gelation Theory”
Supervisor: Prof KOHJIYA, Shinzo
23 March 2006

OGINO, Yoshiko
D Eng, Kyoto University
“Crystallization of Polymers under Shear Flow”
Supervisor: Prof KANAYA, Toshiji
23 May 2006

OHNISHI, Toshiyuki
D Agr, Kyoto University
“Studies on Cytochromes P450 in Brassinosteroid Biosynthesis and Catabolism”
Supervisor: Prof SAKATA, Kanzo
23 May 2006

SAIGO, Hiroto
D Inf, Kyoto University
“Local Alignment Kernels for Protein Homology Detection”
Supervisor: Prof AKUTSU, Tatsuya
24 July 2006

SHIGEOKA, Nobuyuki
D Sc, Kyoto University
“Investigation of Satellites Associated with Fe and Ti K Fluorescence X-ray Emission Spectra”
Supervisor: Assoc Prof ITO, Yoshiaki
23 March 2006

SHIMIZU, Daisuke
D Sc, Kyoto University
“Synthesis of Novel Polythioether Ligands Bearing Substituents and Their Applications to the Synthesis of the Transition Metal Complexes”
Supervisor: Prof TOKITOH, Norihiro
23 March 2006

SHIRAISHI, Yasuhisa
D Pharm Sc, Kyoto University
“Creation of Functional Zinc Finger Proteins Based on the Structure”
Supervisor: Prof FUTAKI, Shiroh
23 March 2006

SUGIYAMA, Yusuke
D Sc, Kyoto University
“Studies on the Low-coordinated Species of Heavier Group 14 Elements Utilizing Kinetic Stabilization”
Supervisor: Prof TOKITOH, Norihiro
23 March 2006

TAKAKURA, Tomoaki
D Agr, Kyoto University
“Industrial Production and Characterization of L-Methionine γ -Lyase, A Potent Antitumor Agent”
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2006

YAMADA, Ikuya
D Sc, Kyoto University
“High Pressure Synthesis and Physical Properties of Oxychloride Superconductors”
Supervisor: Prof TAKANO, Mikio
23 March 2006

YAMADA, Takuji
D Sc, Kyoto University
“Extraction of Phylogenetic Network Modules from the Metabolic Network”
Supervisor: Prof KANEHISA, Minoru
24 July 2006

YAMAZAKI, Atsushi
D Sc, Kyoto University
“Quasi-Monoenergetic Electron Beam by Intense Short Pulse Laser Plasma Interaction”
Supervisor: Prof NODA, Akira
23 May 2006

YOSHIKAWA, Chiaki
D Eng, Kyoto University
“Fundamental and Applied Studies on Living Radical Polymerization”
Supervisor: Prof FUKUDA, Takeshi
23 March 2006



THE 106TH
ICR ANNUAL
SYMPOSIUM

SEMINARS

MEETINGS AND
SYMPOSIA



THE 106TH ICR ANNUAL SYMPOSIUM

(15 December 2006)

ORAL PRESENTATIONS

YAMAGO, Shigeru (Polymer Controlled Synthesis)
“Development of Organobismuthine-Mediated Living Radical Polymerization”

NAKASE, Ikuhiko (Biofunctional Design-Chemistry)
“Arginine-rich Peptide: Recognition of Proteoglycans and Effective Cellular Uptake”

HASHIDA, Masaki (Laser Matter Interaction Science)
“Nano Ablation of Carbon Nanotube Cathode by Femtosecond Laser”

MIZUTANI, Masaharu (Chemistry of Molecular Biocatalysts)
“Diversity of Cytochrome P450 Monooxygenases and Chemical Evolution in Plants”

– ICR Award for Young Scientists –
SASAMORI, Takahiro (Organoelement Chemistry)
“Doubly Bonded Compounds between Heavier Group 15 Elements”

KASAI, Shinya (Nanospintronics)
“Current-Driven Resonant Excitation of Magnetic Vortices”

– ICR Award for Graduate Students –
HIMENO, Atsushi (Nanospintronics)
“Domain Wall Ratchet Effect Induced by an Electric Current”

– ICR Grants for Young Scientists –
KOBAYASHI, Kensuke (Nanospintronics)
“Spin-dependent Transport through Ferromagnetic Nano-particles”

TSUJI, Hayato (The University of Tokyo, Former: Organic Main Group Chemistry)
“Effect of the Molecular Structure and Movement on the Photoelectron Transfer through Silicon Chain”

MATSUDA, Kazunari (Photonic Elements Science)
“Creation of Organic Spintronics Devices Using Carbon Nanotubes”

YOSHIDA, Hiroyuki (Molecular Aggregation Analysis)
“Structure of Organic Layers and Metal/organic Interfaces Inorganic Semiconductor Devices”

MIHARA, Hisaaki (Molecular Microbial Science)
“Exploration of the 23rd Amino Acid by a Collaborative Research of Bioinformatics and Biochemistry”

POSTER PRESENTATIONS

 : Laboratory Whole Presentation
 : Laboratory Topic
 : General Presentation

— Organoelement Chemistry —

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

 ISOBE, Toru; TAKEDA, Nobuhiro; TOKITOH, Norihiro
“Synthesis of Novel Polychalcogenoether Ligands Tethered with Bulky Substituents and Its Application toward the Complexation with Transition Metals”

 MATSUMOTO, Takeshi; SASAMORI, Takahiro; TOKITOH, Norihiro
“Electrochemical Properties of Kinetically Stabilized Sila-aromatic Compounds”

 NAGAHORA, Noriyoshi; SASAMORI, Takahiro; TOKITOH, Norihiro
“Reactions of a Kinetically Stabilized 1,1'-Bis(diphosphanyl)ferrocene with Group 6 Metals”

— Structural Organic Chemistry —

 YOSHIDA, Ryohei; MURATA, Yasujiro; KITAGAWA, Toshikazu
“Generation and Trapping of Phenylated C₆₀ Cation”

 TANABE, Fumiyuki; MURATA, Michihisa; MURATA, Yasujiro
“Encapsulation of Molecular Deuterium inside an Open-Cage C₆₀”

 CHUANG, Shih-Ching; MURATA, Michihisa; MURATA, Yasujiro
“Fine Tuning of the Orifice Size: Synthesis and Properties of Selenium-containing Open-cage C₆₀”

— Synthetic Organic Chemistry —

 TSUBAKI, Kazunori; TAKAISHI, Kazuto; TANAKA, Hiroyuki; MIURA, Masaya; SUE, Daisuke; KAWABATA, Takeo
“Determination of Axial Chirality and Optical Properties of Helical Oligonaphthalenes”

 YOSHIMURA, Tomoyuki; KAWABATA, Takeo
“Enantioselective Total Synthesis of Trolox via Memory of Chirality”

— **Advanced Inorganic Synthesis** —

- GE KAWAI, Masanori; KAN, Daisuke; ISOJIMA, Seiichi; KURATA, Hiroki; SHIMAKAWA, Yuichi
“Structural Characterization of Epitaxial BaTiO₃ Thin Films by Synchrotron X-ray Diffraction and STEM”

— **Chemistry of Polymer Materials** —

- LT ARITA, Toshihiko; OHNO, Kohji; TSUJII, Yoshinobu; FUKUDA, Takeshi
“Developments of Concentrated Polymer Brush”
- GE GAO, Weiping; OHNO, Kohji; TSUJII, Yoshinobu; FUKUDA, Takeshi
“Phase Transition of Well-Defined Concentrated Poly(N-isopropylacrylamide) Brushes in Water”

— **Polymer Controlled Synthesis** —

- GE KOBAYASHI, Yu; YAMAGO, Shigeru
“Organotellurium Mediated Stereocontrolled Living Radical Polymerization of N-isopropyl (Meth)acrylamides”
- GE TOGAI, Manabu; PAN, Na; YAMADA, Takeshi; YAMAGO, Shigeru
“Synthesis of End-Functionalized Polymers Based on Reaction with Azocompounds and Distibine”
- GE TAKEMURA, Kazunobu; YAMAGO, Shigeru
“A Efficient Strategy for the Synthesis of Chondroitin by Iterative Glycosylation”

— **Inorganic Photonics Materials** —

- LW “Recent Topics in Yoko Laboratory”
- LT UEMURA, Koji; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu
“Formation of Two-dimensionally-structured TiO₂ Film by the Photopolymerization-induced Phase Separation in the TiO₂ Colloid - Photosensitive Monomer Coexisting System”

— **Nanospintronics** —

- LW “Research on Nano Spintronics: 2006”
- GE DELMO, Michael P; TAMADA, Yoshinori; YAMAMOTO, Shinpei; TAKANO, Mikio; KASAI, Shinya; KOBAYASHI, Kensuke; ONO, Teruo
“Tunneling Magnetoresistance in FePt Nanoparticles”
- GE TAMADA, Yoshinori
“Synthesis and Easy Axis Alignment of L1₀-FePt Nanoparticles”
- GE YANO, Kuniaki
“The Correlation between Threshold Current Density and Pinning Potential on Current-driven Domain Wall Motion”

— **Biofunctional Design-Chemistry** —

- LT NOSHIRO, Daisuke; TONO, Syunsuke; FUTAKI, Shiroh
“Transmission of Extramembrane Conformational Change into Current: Construction of Metal-gated Ion Channel”
- GE YAN, Wei; IMANISHI, Miki; FUTAKI, Shiroh
“Distinction of Target DNA Phases by a Designed 6-Zinc Finger Peptide with α Helical Linker”

— **Chemistry of Molecular Biocatalysts** —

- LT SHIMIZU, Bun-ichi; KAI, Kosuke; MIZUTANI, Masaharu; KAWAMURA, Naohiro; YAMAGUCHI, H; SAKATA, Kanzo
“Biosynthetic Pathway of Coumarins in Arabidopsis thaliana”
- GE TAI, Liz; HIRATAKE, Jun; MIZUTANI, Masaharu; SHIMIZU, Bun-ichi; SAKATA, Kanzo
“Inhibitors of IAA-Amino Acid Conjugate Synthetases and Hydrolases as Chemical Probes to Study IAA Homeostasis”
- GE NAKAGAWA, Yuichi; HASEGAWA, Atsuko; HIRATAKE, Jun; SAKATA, Kanzo
“Directed Evolution of Lipase for Amide Hydrolysis”
- GE CHO, Jeong-Yong; MIZUTANI, Masaharu; SHIMIZU, Bun-ichi; SAKATA, Kanzo
“Gene Expression Profiling and Chemical Profiling during the Manufacturing Process of Formosa Oolong Tea ‘Oriental Beauty’”

— **Molecular Biology** —

- LT AKI, Shiori; OKA, Atsuhiko; TSUGE, Tomohiko
“The Novel Function of COP9 Signalosome Regulation”

— **Chemical Biology** —

- GE SHIMOGAWA, Hiroki; UESUGI, Motonari
“A Study of Transcriptional Activation with Wrenchnolol Derivatives”

— **Molecular Materials Chemistry** —

- LW “Structure and Dynamics of Functional Molecular Materials”

— **Hydrospheric Environment Analytical Chemistry** —

- LT MOCHAMAD, Lutfi Firdaus; NORISUYE, Kazuhiro; SOHRIN, Yoshiki
“Dissolved and Acid-dissolvable Zr, Hf, Nb, Ta, Mo and W in the Western North Pacific Ocean”
- GE MINAMI, Tomoharu; URUSHIHARA, Shohei; SHIMIZU, Akiyoshi; NAKAGAWA, Yusuke; SOHRIN, Yoshiki
“Comparison of Chelating Absorbents for Separation and Determination of Trace Metals in Seawater”

— **Solution and Interface Chemistry** —

- LT WAKAI, Chihiro
“NMR Study of Ionic Liquids”

- GE KINOSHITA, Tomoko; OKAMURA, Emiko; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru
“In-situ ^{23}Na -NMR Study of Ion Transport through Phospholipid Bilayers”

— Molecular Microbial Science —

- LT YAMAMOTO, Kentaro; KAWAMOTO, Jun; SATO, Satoshi; KURIHARA, Tatsuo; ESAKI, Nobuyoshi
“Physiological Role of Eicosapentaenoic Acid in Cold Adaptation of a Psychrotrophic Bacterium”
- GE YAMAUCHI, Takae; GOTO, Masaru; UO, Takuma; WU, Huiyuan; YOSHIMURA, Tohru; MIHARA, Hisaaki; KURIHARA, Tatsuo; MIYAHARA, Ikuko; HIROTSU, Ken; ESAKI, Nobuyoshi
“Serine Racemase from *S. pombe*: Properties of Its Modified Form”

— Polymer Materials Science —

- LW “Detailed Structural Analysis of Polymers in a Wide Range of Length and Time”
- LT KAWAI, Takahiko; RAHMAN, Nelly
“Crystallization of Poly(lactic acid)”
- LT OGAWA, Hiroki
“Phase Separation and Dewetting in Polymer Blend Thin Films as Studied by Neutron Reflectivity”
- GE ISEKI, Toru
“Structure Analysis of Organic-inorganic Hybrid Low-melting Glasses as Studied by Light Scattering”

— Molecular Rheology —

- GE SAWADA, Toshiaki; MATSUMIYA, Yumi; WATANABE, Hiroshi
“Constraint Release and Dynamic Tube Dilation in Entangled Blends of Star Polyisoprene”

— Molecular Aggregation Analysis —

- LT MURDEY, Richard; SATO, Naoki
“Structure and Electronic Structure of Unoccupied States in Pentacene Thin Films Deposited at Different Substrate Temperatures”
- GE ASAMI, Koji; OKAZAKI, Takashi; NAGAOKA, Yasuo
“Ion Channels of N-Terminally-Linked Alamethicin Dimers”

— Supramolecular Biology —

- LW “Research Activity at Supramolecular Biology”
- GE KATO, Utako; INADOME, Hironori; UMEDA, Masato
“Membrane Phospholipid Dynamics and Its Role in Regulation of Cell Motility”
- GE TAKEUCHI, Ken-ichi; TAKAHARA, Keigo; ISODA, Yuka; UMEDA, Masato
“The Molecular Mechanisms of Temperature Preference in *Drosophila*”

— Particle Beam Science —

- LT IKEGAMI, Masahiro; NODA, Akira; SHIRAI, Toshiyuki; TONGU, Hiromu; TANABE, Mikio; SOUDA, Hikaru
“Generation of Ultra-low-temperature Beams by Laser Cooling”
- GE SHIRAI, Toshiyuki
“String Ion Beam Generation by Electron Cooling”

- GE TONGU, Hiromu; NODA, Akira; SHIRAI, Toshiyuki; IKEGAMI, Masahiro; FUJIMOTO, Shinji; TANABE, Mikio; SOUDA, Hikaru
“Measurement of Beam Lifetime in S-LSR”

— Electron Microscopy and Crystal Chemistry —

- LW “Recent Research Topics in the Division of Electron Microscopy and Crystal Chemistry”
- GE TSUJIMOTO, Masahiko; KURATA, Hiroki; NEMOTO, Takashi; ISODA, Seiji
“Si L_3 -edge ELNES and Threshold Energy for Si and Its Related Materials Calculated by First Principles Band Calculation”
- GE YOSHIDA, Kaname; KAMIYA, Shoko; SHIMIZU, Toshimi; ISODA, Seiji
“A Formation of Self-Assembled Glycolipid Nanotube with Bilayer Sheets”
- GE YAJI, Toyonari; YOSHIDA, Kaname; NEMOTO, Takashi; KURATA, Hiroki; ISODA, Seiji
“STM and STS Study on Pt-chains in bis(1,2-benzoquinone-dioximato) Platinum(II) Thin Films”

— Structural Molecular Biology —

- LT FUJII, Tomomi; HATA, Yasuo
“Crystal Structures of Protein Molecules from Thermophilic and Psychrophilic Bacteria”

— Organic Main Group Chemistry —

- GE ITO, Shingo; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
“Development of Some C-C Bond Formations Exploiting Unreactive Haloalkanes”

— Advanced Solid State Chemistry —

- LT OKA, Kengo
“Charge and Magnetic Orderings in Triangular Lattice Antiferromagnet InFe_2O_4 ”

— Organotransition Metal Chemistry —

- LT MUTOH, Yuichiro; MURAKAMI, Hiromi; HAYASHI, Kyohei; OKAZAKI, Masaaki; OZAWA Fumiyuki
“Highly Reactive Catalysts Bearing Low Coordinate Phosphorus Ligand”

GE TAKANO, Masato; YOSHIMURA, Ken-ichi; OKAZAKI, Masaaki; OZAWA, Fumiyuki
“Redox Switchable Isomerization of Fe₄C₄ Clusters”

— **Photonic Elements Science** —

LW “Recent Research Topics in Photonic Elements Science”

— **Bioknowledge Systems** —

LW “KEGG: the Integrated Database for Genomic and Chemical Information”

— **Biological Information Networks** —

GE TAMURA, Takeyuki; AKUTSU, Tatsuya
“Approximation Algorithms for Optimal RNA Secondary Structures Common to Multiple Sequences”

— **Pathway Engineering** —

LI WAN, Raymond; TAKIGAWA, Ichigaku; MAMITSUKA, Hiroshi
“Extending Splitting Criteria for Classifying Microarray Expression Data”

— **Bioinformatics Training Unit** —

GE ICHIHARA, Hisako; KUMA, Kei-ichi; TOH, Hiroyuki
“Positive Selection in the CSP-ComD System of Streptococcal Species”

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

GE TERASHIMA, Takahito
“Recent Research Activities in Research Center for Low Temperature and Materials Sciences”

SEMINARS

- Dr AMEDURI, Bruno
Ecole Nationale Supérieure de Chimie de Montpellier, France
“Recent Advances in the Controlled Radical Polymerization of Fluorinated Monomers”
1 September 2006
- Prof BALTA-CALLEJA, Francisco J
Instituto de Estructura de la Materia, CSIC, Spain
“Structure Development in Confined Polymer Systems Using X-ray Diffraction Techniques and Nanoindentation Methods”
30 June 2006
- Prof BECKHAM, W. Haskell
Georgia Institute of Technology, USA
“NMR Studies of Cyclic and Threaded Macromolecules”
28 November 2006
- Prof BEPPU, Teruhiko
Nihon University, Tokyo, Japan
“Chemical Approaches to Understanding Biology”
5 October 2006
- Prof BEREK, Dusan
Polymer Institute of the Slovak Academy of Sciences, Slovakia
“Progress in Liquid Chromatography in Synthetic Polymers”
14 April 2006
- Dr BORDNER, Andrew J
Oak Ridge National Laboratory, USA
“Learning from Structure: Predicting Protein-Protein Interfaces and Peptide-MHC Binding Affinities”
30 March 2006
- Prof CHEN, Lih-Juann
Department of Materials Science and Engineering, National Tsing-Hua University, Taiwan
“In-situ Ultrahigh Vacuum Transmission Electron Microscope Investigations of Nanostructures on Silicon”
1 August 2006
- Prof CHO, Hyung-Taeg
Department of Biology, Chungnam National University, Korea
“PINOID Positively Regulates Auxin Efflux from the Cell”
26 May 2006
- Prof CHOU, Li-Jen
National Tsing-Hua University, Taiwan
“Refractory Silicides Nanowires: Interconnect and/or Contact for Future Nanoelectronics and Nanosystems”
12 January 2006
- Prof CRICH, David
University of Illinois at Chicago, USA
“Diastereoselective Glycosylation: Recent Advances”
19 December 2006
- Prof DEVILLANOVA, Francesco A
Departamento di Chimica Inorganica ed Analitica, Università degli Studi di Cagliari, Italy
“The Nature of the Chemical Bond in Linear Three-body Systems: from I_3^- to Mixed Chalcogen/Halogen and Trichalcogen Moieties”
4 October 2006
- Dr DIETRICH, Jürgen
Forschungszentrum Jülich, Germany
“New Experimental Results on Electron Cooling at COSY-Jülich”
7 June 2006
- Dr DREISS, Cecile A
King's College, University of London, UK
“Mixture of Polymers and Small Molecules: Assembling and De-assembling”
18 July 2006
- Prof ELIESER, Shalom
Soreq N. R. C., Yavne, Israel
Madrid Polytechnic University, Madrid, Spain
“Nanoparticles Induced by Femtosecond Lasers”
19 December 2006
- Prof FURUKAWA, Yasu
Nihon University, Graduate School of Bioresource Sciences, Kanagawa, Japan
“History of Polymer Chemistry”
3 August 2006
- Prof GANGULY, Tapan
Department of Spectroscopy, Indian Association for the Cultivation of Science, India
“Attempts for the Productions of Longer-lived Charge Separated Species within Model Donor-acceptor Systems. Compounds of Artificial Photosynthesis and Solar Energy Conversion”
23 August 2006
- Prof GAUVIN, Raynald
Department of Mining, Metals & Materials Engineering, McGill University, Canada
“X-Ray Microanalysis in the Electron Microscope”
23 August 2006
- Prof HIGGINS, Julia S
Imperial College, UK
“Phase Separation in Real and Reciprocal Space”
27 March 2006
- Assoc Prof HIRATA, Takafumi
Graduate School of Science and Engineering, Tokyo Institute of Technology, Tokyo, Japan
“Advance in Mass Spectrometry for Elemental and Isotopic Analysis: Application to Geochemistry and Biochemistry”
6 October 2006

- Dr HORVATH, Tamas
Department of Computer Science III, The University of Bonn, Germany
“Mining and Learning from Graph Structured Data”
9 June 2006
- Prof HWANG, Ildoo
Department of Life Sciences, Pohang University of Science and Technology, Korea
“Recent Progress in Understanding of Cytokinin-Mediated Developmental Control in *Arabidopsis*”
26 May 2006
- Dr ISONO, Erika
Graduate School of Science, The University of Tokyo, Tokyo, Japan
“Spatial-temporal Analysis in Formation and Localization of the 26S Proteasome”
18 May 2006
- Dr ITO, Toshihiko
Toray Research Center, Japan
“Electron Tomography”
13 January 2006
- Prof JAIN, Himanshu
Lehigh University, USA
“Organic-inorganic Hybrid Materials as a Novel Ionic Conductor”
25 July 2006
- Prof KHOMSKII, Daniel I
II Physikalisches Institut, Universitaet zu Koeln, Germany
“Orbitally-Driven Superstructures and Spin Gaps in Spinels and Other Oxides”
14 August 2006
- Dr KIKUTANI, Eiji
High Energy Accelerator Research Organization (KEK), Ibaraki, Japan
“KEKB and Its Future Plan Super KEKB”
14 December 2006
- Prof KIM, Gyung-Tae
Division of Plant Biotechnology, Dong-A University, Korea
“Genetic Analysis of DRL1 (Elongator-Associated Protein) and Holo-Elongator Subunits in *Arabidopsis*”
26 May 2006
- Prof KITAHARA, Takeshi
Teikyo Heisei University, Tokyo, Japan
“Lessons from the History of ‘MONOZUKURI’”
22 June 2006
- Prof KLEIN, Michael L
Laboratory for Research on the Structure of Matter, University of Pennsylvania, USA
“Nothing Amuses More Harmlessly Than Computation ...”
16 June 2006
- Dr KONOKI, Keiichi
Graduate School of Science, Osaka University, Toyonaka, Japan
“Studies on Structure and Function of the Voltage-gated Sodium Channels in *Mya arenaria* Resistant to Paralytic Shellfish Poisoning”
20 July 2006
- Prof KOTORA, Martin
Department of Organic and Nuclear Chemistry, Faculty of Science, Charles University, Praha, Czech R.
“Relation between Cleavage and Formation of C-C Bonds”
9 November 2006
- Prof KRIVANEK, Ondrej
Nion, USA
“Probing Atoms In-situ by Aberration-corrected Scanning Transmission Electron Microscopy”
11 September 2006
- Prof KURODA, Reiko
Graduate School of Arts and Sciences, The University of Tokyo, Japan; A Executive Member of Council for Science and Technology Policy, Japan
“The Third Science and Technology Basic Plan—Fundamental Research, Universities and Innovation”
29 September 2006
- Prof LI, Yuan-Hui
School of Ocean and Earth Science and Technology, University of Hawaii, USA
“Conversion of Organic Nitrogen into N₂ in the Ocean. Where Does It Happen and How?”
3 April 2006
- Prof LIN, King-Fu
Department of Materials Science and Engineering, National Taiwan University, Taiwan
“Fabrication of the Organic/Inorganic Hybrid Nanostructures via Self-assembly of Amphiphilic Light Emitting Molecules”
2 June 2006
- Prof LIU, Hung-wen
College of Pharmacy, University of Texas at Austin, USA
“Learning Nature’s Strategies for Making Unusual Sugars”
6 July 2006
- Prof MA, Shengming
Shanghai Institute of Organic Chemistry, China
“Control of Regio- and Stereoselectivity of Electrophilic Addition of Allenes”
8 November 2006
- Prof MAI, Trong Nhan
VNU, Vietnam
“PCB Distribution in Vietnam Coastal Areas and Its Significance for Environmental Chemistry and Geochemistry”
2 December 2006
- Dr MATSUZAKI, Teiichiro and Dr WATANABE, Isao
Nishina Center, RIKEN, Saitama, Japan
“Muon Studies on Solid State Physics at the RIKEN-RAL Muon Facility—For Collaborating between ICR and RIKEN”
5 October 2006
- Prof MCNAMARA, Pam
Optical Fibre Technology Centre, University of Sydney, Australia
“Black Art to Semi-science—Glass-Making for Photonics—”
16 October 2006
- Prof MESHKOV, Igor N
Joint Institute for Nuclear Research, Dubna, Russia
“New Advances in Beam Cooling”
7 June 2006

Prof MICHL, Josef
University of Colorado at Boulder, USA
“Advances in the Organic Chemistry of Carborane Anions and Radicals”
29 May 2006

Prof MILES, Mervyn John
Physics Department, University of Bristol, UK
“Video-rate AFM”
12 September 2006

Assoc Prof MORITA, Akihiro
Research Center for Computational Science, Institute for Molecular Science, Aichi, Japan
“Theory of Sum Frequency Generation Spectroscopy”
26 January 2006

Prof MUIR, Thomas
Biochemistry and Structural Biology, Rockefeller University, USA
“Assembling and Disassembling Proteins with Light”
9 November 2006

Prof NAGAO, Yoshimitsu
The University of Tokushima, Tokushima, Japan
“Asymmetric Induction Based on Non-Covalent Interactions”
26 July 2006

Prof NAKATANI, Yoshinobu
University of Electro-Communications, Japan
“Simulation of the Current-Induced Domain Wall Motion”
28 April 2006

Dr OKANO, Yasuaki
Institute of Laser Engineering, Osaka University, Japan
“Generation of Quantum Beam Induced by Femtosecond Laser and Its Application”
30 August 2006

Prof OZAKI, Norio
Graduate School of Medicine, Nagoya University, Nagoya, Japan
“Understanding Mental Disorders”
11 August 2006

Prof PARK, Je-Geun
Physics Department, Sung Kyun Kwan University, Korea
“Exploring New States of Matter Using Neutron Scattering”
18 August 2006

Prof PAULUS, Werner
Université de Rennes 1, France
“Non-stoichiometric Oxides”
21 July 2006

Dr PIODA, Alessandro
The University of Tokyo, Japan
“Local Spectroscopy of Quantum Dots”
1 December 2006

Dr PYUN, Jeffrey
University of Arizona, USA
“Magnetic Nanocomposites Composed of Metallic Colloids and Functional Polymer”
14 April 2006

Prof QU, Li-Jia
College of Life Science, Peking University, China
“Auxin Methylation and Leaf Development”
10 August 2006

Prof RUANO, Garcia
Universidad Autonoma de Madrid, Spain
“Stereocontrolled Reactions Mediated by Remote Sulfoxides: Formation and Reactivity of Enantiomerically Pure Benzylic Centers”
21 August 2006

Dr SAITO, Kenji
High Energy Accelerator Research Organization (KEK), Ibaraki, Japan
“Development of Superconducting Rf Cavity at ILC”
14 September 2006

Dr SCHAPER, Andreas
Material Sciences Centre, Philipps University of Marburg, Marburg, Germany
“Structure Evaluation of Radiation-Sensitive Nanosized Materials Using Low-Dose and Cryo-Electron Microscopy”
25 September 2006
“Scrolls—A Special Type of Carbon Nanostructures”
27 September 2006

Prof SCHAUMANN, Ernst
Technical University of Clausthal, Germany
“Silicon Migration as a Useful Tool in Organic Synthesis”
30 August 2006

Prof SCHRAUZER, N. Gerhard
University of California, San Diego, USA
“The Mechanism of Biological Nitrogen Fixation”
7 December 2006

Prof SCHULTZ, G. Peter
The Scripps Research Institute, USA
“New Opportunities at the Interface of Chemistry and Biology”
16 November 2006

Prof SESSLER, Andrew M
Lawrence Berkeley National Laboratory, USA
“A Century of Particle Accelerators”
1 November 2006

Prof SHEVELKO, Viatcheslav P
P. N. Lebedev Physical Institute, Russia
“Works on Atomic Physics Being Done at HIMAC (Chiba) and Lebedev Physical Institute (Moscow)”
20 November 2006

Prof SHISHIDO, Kozo
The University of Tokushima, Tokushima, Japan
“Total Synthesis of Hybrid Natural Products with Biological Activity”
26 July 2006

Dr SMIRNOV, Alexander V
Joint Institute for Nuclear Research, Dubna, Russia
“Simulation of Crystalline Beams in Storage Rings Using Molecular Dynamics Technique”
30 January 2006
“Dependence of Cooling Time on Dispersion in Electron Cooling Section”
2 February 2006

Prof SMOLA, Alex J.
National ICT Australia, Australia
“Maximum Mean Discrepancy for Distribution Testing”
13 October 2006

Prof STROBL, Gert
Physicalisches Institut, Albert-Ludwigs-Universitaet, Germany
“A Multiphase Scheme Treating Polymer Crystallization and Melting”
24 April 2006

Prof STUDER, Armido
Westfälische Wilhelms University, Germany,
“Nitroxides in Synthesis, Polymer Chemistry, and for the Modification of Surfaces”
23 October 2006

Vice-Director TABATA, Satoshi
Kazusa DNA Research Institute, Chiba, Japan
“Molecular and Genetic Analyses by DNA Markers of Leguminous Plants”
23 March 2006

Dr TANAKA, Hirofumi
Research Center for Molecular-scale Nanoscience, Institute for Molecular Science, Japan
“Fabrication of Nanostructure and Nano-device by Organic Molecules”
18 July 2006

Assoc Prof TAUNTON, Jack
Cellular & Molecular Pharmacology, University of California, San Francisco, USA
“Chemical Inhibitors of Signaling and Secretion: Intelligent Design vs. Natural Selection”
26 July 2006

Prof THIERRY, Annette
Institute Charles Sadron, CNRS, France
“Investigation of Twinned Single Crystals of Isotactic Poly(vinyl-cyclohexane) via Electron Microscopy”
12 September 2006

Prof Em TOKUMARU, Katsumi
Department of Chemistry, Graduate School of Science, University of Tsukuba, Tsukuba, Japan
“Room Temperature Phosphorescence EL Materials”
7 December 2006

Dr TURAN, Gyorgy
University of Illinois at Chicago, USA
“Remarks on Learning and Commonsense Reasoning”
9 June 2006

Prof URABE, Shinji
Graduate School of Engineering Science, Osaka University, Osaka, Japan
“Ion Trap and Laser Cooling and Their Applications”
28 July 2006

Dr WANG, Xuhui
Delft University of Technology, Delft, The Netherlands
“Magnetization Dynamics in Metallic Nano-Structures”
28 August 2006

Prof WATANABE, Junji
Tokyo Institute of Technology, Tokyo, Japan
“Study on Biological Nano-scaled Periodical Structures and Their Use for Materials Science”
25 July 2006

Prof WATANABE, Naoharu
Department of Applied Biological Chemistry, Faculty of Agriculture, Shizuoka University, Shizuoka Japan
“Floral Scent Synthesis and Emission in Plants”
13 November 2006

Prof WOLF, Bernhard
University of Mainz, Germany
“Polymer/Polymer Interaction: Consistent Modeling in Terms of Chain Connectivity and Conformational Response”
14 April 2006

Dr WU, Ming-Chien
Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan
“Polymorphism, Crystal Phase Transition and Spherulite Patterns in Semicrystalline Polyesters: Poly(butylene adipate) and Poly(heptamethylene terephthalate)”
1 July 2006

Prof YAMAMURA, Syousuke
Keio University, Tokyo, Japan
“Crosstalk between Biology and Natural Product Chemistry”
27 April 2006

Prof ZHANG, Ze
Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, China
“High Resolution Electron Microscopy Study of Some Low-dimensional Materials”
26 September 2006

MEETINGS AND SYMPOSIA

Nanotechnology Support Project

“Nanotechnology · Nanoscience Focused on Molecules and Materials, IV”

Organized by ISODA, Seiji
14–15 March 2006 (Kyoto, Japan)

21st Century COE on Kyoto University Alliance for Chemistry **“Chemical Biology Symposium”**

Organized by FUTAKI, Shiroh; SUGIYAMA, Hiroshi; HAMACHI, Itaru
15–16 March 2006 (Kyoto, Japan)

Special Lectures on Bioinformatics

Organized by Education and Research Organization for Genome Information Science (Leader: KANEHISA, Minoru)
24 June 2006 (Kyoto, Japan)

Dr BORK, Peer

European Molecular Biology Laboratory, Germany
“Predicting Biological Function at Different Scales”

Dr BRYANT, Steve

National Center for Biotechnology Information, USA
“CDD: NCBI’s Protein Family/subfamily Classification Database”

Prof ELLIS, Lynda

University of Minnesota, USA
“Seeking the Vertebrate Secretome”

Dr SHMULEVICH, Ilya

Institute for Systems Biology, USA
“Eukaryotic Cells Are Dynamically Ordered or Critical but Not Chaotic”

Prof PRINT, Cristin

University of Auckland, New Zealand
“What Can the Transcriptome Tell Us About Blood Vessel Walls?”

Prof SCHOMBURG, Dietmar

University of Koeln, Germany
“From Enzyme Classification and Metabolome Research to Systems Biology”

2006 Regional Meeting of Japanese Society of Microscopy, **“Kansai Branch”**

Organized by ISODA, Seiji
15 July 2006 (Kyoto, Japan)

21st Century COE on Kyoto University Alliance for Chemistry **“ICR Biofunctional Chemistry Seminar”**

Organized by KAWABATA, Takeo; FUTAKI, Shiroh
3 August 2006 (Uji, Japan)

Cyanobacteria Annotatoin Workshop

Organized by KANEHISA, Minoru
22–23 August 2006 (Kyoto, Japan)

The 56th Symposium on Coordination Chemistry of Japan **“Synergistic Effects for Creation of Functional Complexes”**

Organized by OKAZAKI, Masaaki
16 September 2006 (Hiroshima, Japan)

Prof MIYAURA, Norio
Hokkaido University

Prof NAKAZAWA, Hiroshi
Osaka City University

Prof UENO, Keiji
Gunma University

Dr TSUBOYAMA, Akira
CANON Inc.

Prof SEKIGUCHI, Akira
University of Tsukuba

20th Anniversary (40th) Symposium of the Solid-State NMR **for Materials**

Organized by HORII, Fumitaka; KAJI, Hironori et al.
16–17 October, 2006 (Kyoto, Japan)

21st Century COE on Kyoto University Alliance for Chemistry **“The 3rd Organoelement Chemistry Seminar”**

Organized by TOKITOH, Norihiro; OZAWA, Fumiyuki; SASAMORI, Takahiro; NAGAHORA, Noriyoshi
26 October 2006 (Kyoto, Japan)

A Satellite Meeting of International Conference of 43rd **Japanese Peptide Symposium/4th Peptide Engineering** **Meeting**

“Membrane-Permeable Peptides: Chemistry, Biology and Therapeutic Applications”

Organized by FUTAKI, Shiroh; MATSUZAKI, Katsumi; MORII, Takashi; NAGASAKI, Takeshi
10–11 November 2006 (Kyoto, Japan)

Kyoto Conference on Solid State Chemistry

“Transition Metal Oxides: – Past Present and Future –”

Organized by TAKANO, Mikio
14–18 November 2006 (Kyoto, Japan)

Dr KANAMORI, Junjiro

International Institute for Advanced Studies, Japan
“Magnetism in Solids—A Crossroads of Chemistry and Physics”

Prof RAO, C. N. R.

Jawaharlal Nehru Centre for Advanced Scientific Research, India
“Transition Metal Oxides: Important Directions”

- Prof AKIMITSU, Jun
Department of Physics and Mathematic, Aoyama-Gakuin University, Japan
“Pursuing Higher-Tc Superconductors—Past, Present and Future—”
- Prof RAVEAU, Bernard
CRISMAT / ENSICAEN, France
“The Impact of Crystal Chemistry upon the Magnetic and Transport Properties of Strongly Correlated Oxide Systems”
- Prof TAKAGI, Hidenori
Department of Advanced Materials, Tokyo University, Japan
“Gate-Induced Phase Change in Transition Metal Oxide Channels”
- Prof ALARIO-FRANCO, Miguel A.
Laboratorio de Química del Estado Sólido, Facultad de Química, Universidad Complutense, Spain
“The Influence of the Microstructure on the Very High Li⁺ Conductivity in LaLiTiO Type of Materials: Ahead of the Structure-Property Relations Paradigm”
- Prof KANNO, Ryoji
Department of Electronic Chemistry, Interdisciplinary School of Science and Engineering, Tokyo Institute of Technology, Japan
“Lithium Ionic Conductor, Thio-LISICON: Materials Design, Conduction Mechanism, and All Solid-State Battery”
- Prof GRENIER, Jean-Claude
I. C. M. C. B.- C. N. R. S., FRANCE
“Mixed Ionic Electronic Conducting Oxides: Advanced Materials for Intermediate Temperature Solid Oxide Fuel Cells”
- Dr SAKABE, Yukio
Murata Manufacturing Co., Ltd., Japan
“Preparation of Nano-Sized BaTiO₃ Powder for Advanced Multilayer Ceramic Capacitors”
- Dr SATO, Ken-ichi
Sumitomo Electric Industries, Ltd., Japan
“Bismuth-based High Temperature Superconducting Wires and Applications”
- Prof CAVA, Robert J.
Department of Chemistry, Princeton University, USA
“Ferromagnetism in Mn-doped BiTe and the Crystal Chemistry of Bismuth Tellurides”
- Prof MAEKAWA, Sadamichi
Institute for Materials Research, Tohoku University, Japan
“Anomalous Electronic Lattices in Cobaltates”
- Prof UEDA, Yutaka
Institute for Solid State Physics, University of Tokyo, Japan
“Have Been Fascinated with Vanadium Oxides”
- Prof ATTFIELD, J. Paul
Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh, UK
“New Surprises in Magnetic Metal Oxides”
- Dr SHIRO, Yoshitsugu
RIKEN Spring-8 Center, Japan
“Redox Chemistry of Hemoproteins”
- Prof TOKURA, Yoshinori
Department of Applied Physics, The University of Tokyo, Japan
“Rich Electronic Phases and Gigantic Response in Transition-Metal Oxides”
- Prof FUJIMORI, Atsushi
Department of Complexity Science and Engineering, The University of Tokyo, Japan
“Oxygen *p*-Hole Character in Transition-Metal Oxides Revealed by Photoemission Spectroscopy”
- Prof GOODENOUGH, J. B.
Texas Materials Institute, ETC 9.102 The University of Texas at Austin, USA
“Orbital Ordering in Perovskites”
- Prof TAKANO, Mikio
Institute for Chemical Research, Kyoto University
“Fe⁴⁺ Oxides”
- Prof POEPELMEIER, Kenneth R.
Northwestern University, Department of Chemistry, USA.
“Enabling Photovoltaic Materials: Rational Syntheses and Properties of Transparent Conductors”
- Prof HOSONO, Hideo
Tokyo Institute of Technology, Frontier Collaborative Research Center, Japan
“Room Temperature Stable Electride: Synthesis, Properties, Electronic Structure, and Application”
- Prof HWANG, Harold Y.
Department of Advanced Materials Science, Department of Applied Physics, The University of Tokyo, Japan
“Chemistry of Oxide Heterointerfaces on the Atomic Scale”
- Prof ITOH, Mitsuru
Materials and Structures Laboratory, Tokyo Institute of Technology, Japan
“Chemical Design for Perovskite-Related Ferroelectrics”
- Prof SHIMAKAWA, Yuichi
Institute for Chemical Research, Kyoto University, Japan
“Transition-metal Oxides with Spin-Polarized Conduction Carriers: Materials and Their Applications”
- Dr KITAZAWA, Koichi
Japan Science and Technology Agency, Japan
“Three Superconducting Global Networks—Towards Renewable Energy Era—”
- Prof BATTLE, Peter
Inorganic Chemistry Laboratory, Oxford University, UK
“Cation and Charge Ordering in Perovskite-Related Structures”
- Assoc Prof SHIMOYAMA, Jun-ichi
Department of Applied Chemistry, The University of Tokyo, Japan
“Oxygen Stoichiometry and Mixed Valence States in Layered Transition Metal Oxides”
- Prof TERASAKI, Ichiro
Department of Applied Physics, Waseda University, Japan
“Unconventional Ferromagnet Sr₃RCO₄O_{10.5}”
- Prof SABRAMANIAN, Mas
Department of Chemistry, Oregon State University, USA
“Designing High Efficiency Thermoelectric Materials for Energy Harvesting: Role of Solid State Chemistry”
- Prof JANSEN, Martin
Max-Planck-Institute for Solid State Research, Germany
“The Family of Si-B-N-C Ceramics: Paving the Way to Industrial Scale Production”

Prof HASHIMOTO, Kazuhiro
Research Center for Advanced Science and Technology, The University of Tokyo, Japan
“Photo-induced Reactions on TiO₂ Surface: Fundamentals and Applications”

Prof YAMANAKA, Shoji
Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Japan
“Chemical Modification and Superconductivity of Layer Structured Transition Metal Nitride Halides”

Prof KAWASAKI, Masashi
Institute for Materials Research, Tohoku University, Japan
“Oxide Electronics Pursuing True Application”

Prof YAN, Chun-Hua
State Key Lab of Rare Earth Materials Chemistry and Applications, Peking University, China
“Controlled Synthesis and Properties of Rare Earth Nanooxides”

Dr TAKAYAMA-MUROMACHI, Eiji
Advanced Nano Materials Laboratory, National Institute for Materials Science, Japan
“Superconducting Phase Diagram of the Sodium Cobalt Oxhydrate”

Prof YOSHIMURA, Kazuyoshi
Department of Chemistry, Graduate School of Science, Kyoto University, Japan
“Systematic Sample Preparation and Characterizations of Superconducting Na_xCoO₂·yH₂O: Anisotropic Knight Shifts and Spin Fluctuations”

Prof HIROI, Zenji
Institute for Solid State Physics, The University of Tokyo, Japan
“Rattling Behavior of Alkali Cations in β-Pyrochlore Oxide Superconductors AOs₂O₆”

Prof FUKUYAMA, Hidetoshi
Department Applied Physics, Faculty of Science, Tokyo University of Science, Japan
“B-doped Diamonds: High Temperature Superconductivity by Transforming Bonds into Bands”

Poster Presentations

Shinsuke Abe, Shiro Kambe and Osamu Ishii
Graduate School of Science and Engineering, Yamagata University, Japan
“Precise Measurement of Na and H₂O Content in Na_xCoO₂·yH₂O”

Mitsuru Akaki, Kohei Noda, Fumiaki Nakamura, Daisuke Akahoshi and Hideki Kuwahara
Department of Physics, Sophia University, Japan
“Competition between Spiral and A-type Antiferromagnetism in Multiferroic RMnO₃ Crystals”

Masaki Azuma, Sandra Carlsson, Jennifer Rodgers, Mathew G. Tucker, Shintaro Ishiwata, J. Paul Attfield, Yuichi Shimakawa and Mikio Takano
Institute for Chemical Research, Kyoto University, Japan
“Pressure Induced Charge Transfer from A to B Sites in a Perovskite BiNiO₃”

Alexei A. Belik, Tadahiyo Yokosawa, Koji Kimoto, Yoshio Matsui and Eiji Takayama-Muromachi
Advanced Nano Materials Laboratory, National Institute for Materials Science, Japan
“High-Pressure Synthesis and Properties of Solid Solutions BiMnO₃-BiScO₃”

A. Crisan, Y. Tanaka, A. Iyo, K. Tokiwa and T. Watanabe
National Institute of Advanced Industrial Science and Technology (AIST), Japan
“Coexistence of Superconductivity and Antiferromagnetism in HgBa₂Ca₄Cu₅O_y Reflected in Vortex Dynamics”

Kais Daoudi, Tetsuo Tsuchiya, Tomohiko Nakajima, Iwao Yamaguchi, Takaaki Manabe and Toshiya Kumagai
Japan National Institute of Advanced Industrial Science and Technology (AIST), Japan
“TEM Study of the La_{0.7}Ca_{0.3}MnO₃ Thin Films Grown on SrTiO₃ Substrate by ELAMOD Process: Formation Mechanism”

Kazuaki Ebata, Hiroki Wadati, Masaru Takizawa, Koji Maekawa, Atsushi Fujimori, Akira Chikamatsu, Hiroshi Kumigashira, Masaharu Oshima, Yasuhide Tomioka, Hideki Kuwahara and Yoshinori Tokura
Department of Complexity Science and Engineering, The University of Tokyo, Japan
“Photoemission Study of Mixed-valence Manganites”

Yosefu Fujiki, Akamatsu Hirofumi, Shunsuke Murai, Koji Fujita and Katsuhisa Tanaka
Industrial Solid State Chemistry Laboratory, Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Japan
“Magnetic and Magneto-optical Properties of Disordered Cadmium Ferrite Thin Films”

Tatsuo Fujii, Miki Yamashita, Shinichi Fujimori, Yuji Saitoh, Tetsuya Nakamura, Keisuke Kobayashi and Jun Takada
Department of Applied Chemistry, Okayama University, Japan
“Fe 3d - Ti 3d Inter-valence Charge Transfer of FeTiO₃”

Naoaki Hayashi, Shigetoshi Muranaka, Takahito Terashima and Mikio Takano
Graduate School of Human and Environmental Studies, Kyoto University, Japan
“Anomalous Phase Transition of SrFeO₃ Studied Using a Single-Crystalline Film”

Shigeto Hirai, Fernando Aguado, Geoffrey Bromiley and Simon Redfern
Department of Earth Sciences, University of Cambridge, UK
“Physical Properties and the Structure of CaIrO₃”

Noriya Ichikawa and Hiroshi Sakama
Department of Physics, School of Science and Technology, Sophia University, Japan
“Growth and Properties of Magneto-electric BiFeO₃ Thin Films”

Masaki Ikeda, Teppei Yoshida, Makoto Hashimoto, Atsushi Fujimori, Masato Kubota, Kanta Ono, Keiichi Unozawa, Takao Sasagawa and Hidenori Takagi
Department of Complexity Science and Engineering and Department of Physics, The University of Tokyo, Japan
“Strong Antiferromagnetic Effects in the Electron-doped High-Tc Superconductor Sm_{2-x}Ce_xCuO₄”

N. Ikeda, S. Mori, Y. Horibe and K. Yoshii
Department of Physics, Okayama University, Japan
“Ferroelectricity of Electronic in RFe₂O₄”

- Yoshinori Imai, Masatsune Kato, Yuichiro Takarabe, Takashi Noji, Tadashi Adachi and Yoji Koike
Nanomaterials Synthesis Group, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Japan
“Low-temperature Synthesis of La_2CuO_4 with the T'-structure Using Molten Hydroxides”
- Yoshiyuki Inaguma and Tetsuhiro Katsumata
Department of Chemistry, Faculty of Science, Gakushuin University, Japan
“Phase Transition of a Perovskite $\text{Bi}(\text{Ni}_{1/2}\text{Ti}_{1/2})\text{O}_3$ ”
- S. Ishiwata, W. Kobayashi, I. Terasaki, K. Kato, M. Takata, Y. Kusano, T. Saito and M. Takano
Waseda University, Japan
“Structure-Property Relation in Sr-Co-O Systems”
- Kenji Tateishi and Nobuo Ishizawa
Ceramics Research Laboratory, Nagoya Institute of Technology, Japan
“Bond-length Fluctuation in the Orthorhombic LiMn_2O_4 —A Possible Existence of Zener-type Polarons—”
- Tsuyoshi Suwa, Nobuo Ishizawa and James R. Hester
Ceramics Research Laboratory, Nagoya Institute of Technology, Japan
“Noncentrosymmetric Polymorph of Partially-Disordered Tb_3RuO_7 ”
- Masahiko Isobe, Shigenori Koishi, Jun-Ichi Yamaura, Toru Yamauchi, Hiroaki Ueda, Hirotada Gotou, Takehiko Yagi and Yutaka Ueda
Institute for Solid State Physics, The University of Tokyo, Japan
“Metal-Insulator Transition in Hollandite $\text{K}_2\text{V}_8\text{O}_{16}$ ”
- Akira Iyo, Yasumoto Tanaka, Yasuharu Kodama, Hijiri Kito, Kazuyasu Tokiwa and Tsuneo Watanabe
National Institute of Advanced Industrial Science and Technology (AIST), Japan
“High-pressure Synthesis of Hg-12(n-1)n Multilayered Cuprates Including up to Fifteen CuO_2 Layers (n=15) in a Unit Cell”
- Cédric Tassel, Hiroshi Kageyama, Yoshitami Ajiro and Kazuyoshi Yoshimura
Department of Chemistry, Graduate School of Science, Kyoto University, Japan
“Single Crystal Growth of the Ion-Exchanged Layered Perovskite $(\text{CuCl})\text{LaNb}_2\text{O}_7$ ”
- Tetsuya Kajita, Masatsune Kato, Takashi Noji and Yoji Koike
Department of Applied Physics, Tohoku University, Japan
“A New Family of Electron-Doped Superconducting Cuprates $\text{Li}_x\text{Sr}_2\text{CuO}_2\text{X}_2$ (X = Br, I)”
- Daisuke Kan, Atsushi Ishizumi, Ryoko Kanda, Atsunobu Masuno, Takahito Terashima, Yoshihiko Kanemitsu, Mikio Takano and Yuichi Shimakawa
Institute for Chemical Research, Kyoto University, Japan
“Blue-Luminescence from Electron-doped Metallic SrTiO_3 ”
- N. Katayama, M. Nohara, M. Uchida and H. Takagi
Department of Advanced Materials Science, The University of Tokyo, Japan
“Metal to Nonmagnetic-Insulator Transition in LiVS_2 ”
- Masatsune Kato, Yoshinori Imai, Tetsuya Kajita, Takashi Noji and Yoji Koike
Department of Applied Physics, Tohoku University, Japan
“Synthesis of Oxide Superconductors by Soft-Chemical Techniques”
- Tetsuhiro Katsumata, Hiroaki Takase, Yoshiyuki Inaguma, Jacques Barbier, John E. Greedan, Lachlan Cranswick and Mario Bieringer
Faculty of Science, Gakushuin University, Japan
“Crystal and Magnetic Structures of Perovskite-type Oxyfluoride, $x\text{PbTiO}_3 - (1-x)\text{PbFeO}_2\text{F}$ ”
- Yasuharu Kodama, Manabu Hirai, Hijiri Kito, Yasumoto Tanaka and Akira Iyo
Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Japan
“Anomalous Dependence of Tc in Multi-layered Cuprate Superconductors of $(\text{Cu,C})\text{Ba}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_x$ (n = 3,4,5,6)”
- Shinji Kono, Naoki Shirakawa, Ichiro Nagai, Norio Umeyama, Kazuyasu Tokiwa and Tsuneo Watanabe
Department of Applied Electronics, Tokyo University of Science, Japan
“The Synthesis and Characterization of a Layered Perovskite $\text{Sr}_2\text{V}_{1-x}\text{Mo}_x\text{O}_4$ ”
- Nobuhiro Kumada, Yoshinori Yonesaki, Takahiro Takei and Nobukazu Kinomura
Department of Research Interdisciplinary, Graduate School of Medicine and Engineering, University of Yamanashi, Japan
“Preparation and Crystal Structure of New Niobium Oxides”
- Yasushi Kurihara and Hirohiko Sato
Department of Physics, Chuo University, Japan
“Magnetism and Conductivity in Calcium Iridate: Ca_2IrO_4 ”
- Chris D. Ling and Karina Aivazian
School of Chemistry, The University of Sydney, Australia
“Crystallographic Investigation of Oxygen Vacancies in the Misfit-layered Cobaltite ‘ $\text{Ca}_3\text{Co}_4\text{O}_9$ ’”
- Atsunobu Masuno, Jianding Yu and Yasutomo Arai
Japan Aerospace Exploration Agency, Institute of Space and Astronautical Science, Japan
“Structural and Physical Properties of BaTi_2O_5 Glasses Prepared by Containerless Processing”
- Daisuke Mori, Noriyuki Sonoyama, Atsuo Yamada, Ryoji Kanno, Masaki Azuma, Mikio Takano, Katsumi Suda and Nobuo Ishizawa
Department of Electronic Chemistry, Interdisciplinary School of Science and Engineering, Tokyo Institute of Technology, Japan
“Single-crystal Growth of $\text{Tl}_2\text{Ru}_2\text{O}_7$ Pyrochlore Using High-pressure and Flux Method”
- S. Mori, S. Shinohara, Y. Matsuo, Y. Horibe, K. Yoshii and N. Ikeda
Department of Physics, Osaka Prefecture University, Japan
“TEM Study of Charge Ordered Structure in $\text{YFe}_2\text{O}_{4-\delta}$ ”
- Hidekazu Mukuda, Yoshio Kitaoka, Shintaro Ishiwata, Takashi Saito, Yuichi Shimakawa, Hisatomo Harima and Mikio Takano
Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Japan
“Stepwise Magnetization and Magnetotransport in $\text{SrCo}_6\text{O}_{11}$ with Metallic Kagomé Layer and Triangular Lattice with Local Moments; ^{59}Co -NMR”

- Taiya Munenaka and Hirohiko Sato
Department of Physics, Chuo University, Japan
“A Novel Metallic Pyrochlore Ruthenate: $\text{Ca}_2\text{Ru}_2\text{O}_7$ ”
- Yuji Muraoka and Zenji Hiroi
The Graduate School of Natural Science and Technology,
Okayama University, Japan
“Persistent Photoconductivity in an SnO_2 Thin Film”
- Yohei Nagao, Jun-Ichi Yamaura and Zenji Hiroi
Institute for Solid State Physics, University of Tokyo, Japan
“Preparation and Superconducting Property of β -pyrochlore
Oxides RbOs_2O_6 and CsOs_2O_6 ”
- Kanako Nakajima and Hirohiko Sato
Institute for Physics, Chuo University, Japan
“A Novel Lithium Ruthenate: Li_8RuO_6 ”
- Tomohiko Nakajima, Tetsuo Tsuchiya and Toshiya Kumagai
Thin Films Processing Group, AMRI, Advanced Industrial
Science and Technology, Japan
“New Route for Low-temperature Fabrication of Perovskite
Titanate Phosphor Thin Film”
- Hiroaki Ueda, Tsuru Yamauchi, Kanji Ohwada, Hajime Sagayama,
Hiroshi Sawa and Yutaka Ueda
Institute for Solid State Physics, The University of Tokyo, Japan
“Devil’s Staircase Behavior of $\beta\text{-Sr}_{0.33}\text{V}_2\text{O}_5$ ”
- Seiji Niitaka, Keisuke Nishikawa, Syotaro Kimura and Yasuo
Narumi, Kouichi Kindo, Masayuki Hagiwara and Hidenori
Takagi
RIKEN (The Institute of Physical and Chemical Research),
Japan
“High-Field Magnetization Study of Heavy Fermion Oxide
 LiV_2O_4 ”
- Minoru Nohara, Hiromichi Kuriyama and Hidenori Takagi
Department of Advanced Materials Science, The University of
Tokyo, Japan
“Thermoelectric Oxide CuRhO_2 ”
- Ippei Nomoto and Hirohiko Sato
Department of Physics, Chuo University, Japan
“Synthesis of a Novel B-Fe-O Compound and Its Metamag-
netism”
- Kenya Ohgushi, Hirotada Gotou, Takehiko Yagi and Yutaka
Ueda
Institute for Solid State Physics, The University of Tokyo, Japan
“Olivine and Post-perovskite Structure as Playground for
Studying Correlated Electronic Properties”
- Daichi Kubota, Tetsuro Tanaka and Katsuyoshi Oh-ishi
Department of Applied Chemistry, Faculty of Science and
Engineering, Chuo University, Japan
“Superconductivity and Magnetic Property of $\text{Ce}_{0.15}\text{Nd}_{1.85-x}\text{Gd}_x\text{CuO}_{4-y}$ 214-n-type Superconductor”
- H. Ohta, C. Michioka, Y. Itoh and K. Yoshimura
Department of Chemistry, Graduate School of Science, Kyoto
University, Japan
“ ^{23}Na NMR Studies of Non-superconducting and Superconduct-
ing $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ ($T_c < 1.8$ and ~ 4.5 K)”
- Yoshihiko Okamoto, Minoru Nohara and Hidenori Takagi
Magnetic Materials Laboratory, RIKEN, Japan
“Spin Liquid State in $\text{Na}_4\text{Ir}_5\text{O}_{13}$ ”
- Paul J. Saines and Brendan J. Kennedy
School of Chemistry, The University of Sydney, Australia
“Electronic Transitions and Oxygen Vacancies in $\text{Ba}_2\text{LnSn}_x\text{Sb}_{1-x}\text{O}_{6-d}$ ”
- Takashi Saito, Anthony Williams, John Paul Attfield, Tuerxun
Wuernisha, Takashi Kamiyama, Shintaro Ishiwata, Yuhki Takeda,
Yuichi Shimakawa and Mikio Takano
Institute for Chemical Research, Kyoto University, Japan
“Spin Frustration in $\text{SrCo}_6\text{O}_{11}$ ”
- Chikako Sakai, Fumihiko Matsui, Nobuaki Takahashi, Sakura
Nishino Takeda and Hiroshi Daimon
Graduate School of Materials Science, Nara Institute of Science
and Technology (NAIST), Japan
“Hybridized Orbital Symmetry Determination of the Fermi
Energy Band of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_y$ Superconductor by Non-
polarized Light Two-dimensional Photoelectron Spectroscopy”
- Hiroya Sakurai and Eiji Takayama-Muromachi
National Institute for Materials Science, Japan
“Soft-Chemical Synthesis and Magnetic Properties of Sodium
Cobalt Oxides”
- Yusuke Sasakawa, Yusuke Nihei and Kunio Okimura
Department of Electronics, Tokai University, Japan
“X-ray Diffraction Study on Electric Field Induced Metal-
Insulator Transition of Vanadium Dioxide Films on Sapphire
Substrate Prepared by Reactive Sputtering”
- S. Iikubo, H. Koyanaka, S. Shamoto, K. Takeuchi, S. Kohara, K.
Kodama and C. -K. Loong
Quantum Beam Science Directorate, Japan Atomic Energy
Agency, Japan
“Local Structural Study of a Manganese Oxide Gold-Adsorbent”
- Neeraj Sharma, Chris D. Ling, Parry Chen and Grant Wrighte
School of Chemistry, Building F11, The University of Sydney,
Australia
“Ruthenium (IV), Iridium (IV) and Manganese (IV) Incorpora-
tion into Three-layer Aurivillius Phases”
- C. T. Shih, Y. C. Chen, H. C. Chien, J. J. Wu and T. K. Lee
Department of Physics, Tunghai University, Taiwan
“Interplay between Antiferromagnetism and Superconductivity
of the Extended t-J Model”
- D. D. Shivagan, A. Sundaresan, A. Crisan, Y. Tanaka, A. Iyo, K.
Tokiwa and T. Watanabe
Superconducting Materials Group, Nanoelectronics Research
Institute, AIST, Japan
“Development of Tl-1223 Films for the Quest of i-solitons”
- Kent Sonoda, Masaaki Fujihara, Naokazu Komiyama, Shiro
Kambe and Osamu Ishii
Human Sensing Program, Graduate School of Science and Engi-
neering, Yamagata University, Japan
“High-pressure Treatment of $\text{InBa}_2\text{CuO}_y$ without Changing
Crystal Structure”
- Jun Takada and Yoshihiro Kusano
Department of Applied Arts and Design, College of the Arts,
Kurashiki University of Science and the Arts, Japan
“Reddish Color Pattern on Traditional Japanese Bizen Stoneware”

- Keitaro Tezuka, Taro Nambo, Shan Yue Jin, Hideo Imoto and Kenji Ohoyama
Department of Applied Chemistry, Faculty of Engineering, Utsunomiya University, Japan
“Crystal Structures and Magnetic Properties of Ln_2CrS_4 (Ln = Y, Ho - Tm)”
- Tetsuya Tohei, Akihito Kuwabara, Fumiyasu Oba and Isao Tanaka
Department of Materials Science and Engineering, Kyoto University, Japan
“First Principles Study of Phonon Instability in REAlO_3 Perovskite Compounds”
- Masashi Tokunaga, Shinya Hakuta and Tsuyoshi Tamegai
Department of Applied Physics, The University of Tokyo, Japan
“Study of Electronic States in Crystals of Bismuth-based Manganites”
- T. Tsuchiya, K. Daoudi, T. Nakajima and T. Kumagai
Japan National Institute of Advanced Industrial Science and Technology (AIST), Japan
“Control of the Electrical Properties of the Epitaxial $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ Thin Film by Excimer Laser Assisted Metal Organic Deposition”
- Naohito Tsujii and Hideaki Kitazawa
National Institute for Materials Science, Japan
“Synthesis and Properties of Quasi-two-Dimensional Triangular-lattice System $\text{CuCr}_{1-x}\text{V}_x\text{S}_2$ ”
- Y. Tsujimoto, Y. Baba, N. Oba, H. Kageyama, Y. Ajiro, K. Yoshimura, T. Saito, M. Takano, Y. Narumi, K. Kindo, G. J. MacDougall, A. Aczel, J. P. Carlo, P. Russo, G. M. Luke and Y. J. Uemura
Department of Chemistry, Graduate School of Science, Kyoto University, Japan
“Magnetization and Heat Capacity of a Layered Perovskite (CuBr) $\text{Sr}_2\text{Nb}_3\text{O}_{10}$ ”
- Atsushi Tsurumaki, Nao Takeshita, Yuji Muraoka, Zenji Hiroi, Hidenori Takagi and Yoshinori Tokura
Institute for Solid State Physics, The University of Tokyo, Japan
“Superconducting Properties of a $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ Thin Film Grown on an Atomically Stepped Substrate”
- Chong Tet Vui and Shiro Kambe
Human Sensing Program, Graduate School of Science and Engineering, Yamagata University, Japan
“Effects of Zn and Ni Substituted $\text{GdBaSrCu}_3\text{O}_{7-\delta}$ Superconductor”
- T. Waki, M. Takigawa, T. Yamauchi, J. Yamaura, H. Ueda and Y. Ueda
Institute for Solid State Physics, The University of Tokyo, Japan
“NMR Study on a Single Crystal of $\beta\text{-Sr}_{0.33}\text{V}_2\text{O}_5$ ”
- Dan Wang and Ranbo Yu
Key Laboratory of Multi-phase Reaction Institute of Process Engineering Chinese Academy of Science, China
“Size and Morphology Control of $\alpha\text{-Fe}_2\text{O}_3$ Particles”
- Satoshi Watauchi, Masashi Fukasawa, Shinsuke Morimoto, Jong Kwan Park, A. T. M. Nazmul Islam and Isao Tanaka
Center for Crystal Science and Technology, University of Yamanashi, Japan
“Effects of Dopant in Molten Zone during Crystal Growth of Rutile by Traveling Solvent Floating Zone Method”
- Takeshi Yajima, Tomohiro Takayama and Hidenori Takagi
Department of Advanced Materials Science, The University of Tokyo, Japan
“Orbital Ordering in NaNiO_2 —towards ‘Orbital’ Refrigeration—”
- H. Yamada, T. Lottermoser, N. Kida, T. Arima, M. Kawasaki and Y. Tokura
Correlated Electron Research Center (CERC), National Institute of Advanced Industrial Science and Technology (AIST), Japan
“‘Tricolor’ Oxide Superlattice as an Artificial Polar Ferromagnet”
- Ikuya Yamada, Masaki Azuma, Kazuki Ohishi, Yuichi Shimakawa and Mikio Takano
Institute for Chemical Research, Kyoto University, Japan
“Single Crystal Growth of Calcium Oxychloride Superconductors $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ and $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$ at High Pressure”
- Ayako Yamamoto and Hidenori Takagi
Magnetic Materials lab., RIKEN (The Institute of Physical and Chemical Research), Japan
“Metal-Semiconductor Transition in $\text{Hg}_2\text{Ru}_2\text{O}_7$ ”
- Shinpei Yamamoto, Yasumasa Morimoto, Yoshinori Tamada, Yukiko Takahashi, Kazuhiro Hono, Teruo Ono and Mikio Takano
Institute for Chemical Research, Kyoto University, Japan
“Synthesis and Magnetic Properties of $\text{Ll}_0\text{-FePt}$ Nanoparticles”
- Jun-Ichi Yamaura, Yohei Nagao and Zenji Hiroi
Institute for Solid State Physics, The University of Tokyo, Japan
“Structural Study of Rattling Cations in the Pyrochlore Oxide Superconductors $\beta\text{-AO}_2\text{O}_6$ (A = K, Rb, Cs)”
- Kazuki Nagashima, Takeshi Yanagida, Hidekazu Tanaka and Tomoji Kawai
Institute of Scientific and Industrial Research (ISIR-Sanken), Osaka University, Japan
“Strain Effects on Metal-Insulator Transition of VO_2 Thin Films”
- Kazuki Nagashima, Takeshi Yanagida, Hidekazu Tanaka and Tomoji Kawai
Institute of Scientific and Industrial Research (ISIR-Sanken), Osaka University, Japan
“MgO Nanowires by Pulsed Laser Deposition”
- Toru Yoshida, Hiroaki Hayamizu, Hiroyuki Yohida and Zenji Hiroi
Institute for Solid State Physics, The University of Tokyo, Japan
“Spinodal Decomposition in $\text{Ti}_x\text{V}_{1-x}\text{O}_2$ ”
- D. Yoshizumi, Y. Muraoka and Z. Hiroi
Institute for Solid State Physics, The University of Tokyo, Japan
“Correlation between Conductivity and Order/Disorder State of Na Ions in Na_xCoO_2 ”
- K. Kugimiya, K. Fujita, K. Tanaka and K. Hirao
Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Japan
“Magnetic and Transport Properties of Oxygen Deficient $\text{EuTiO}_{3-\delta}$ Thin Films Prepared by the PLD Method”
- Nanao, Horiishi
TODA KOGYO CORP., Japan
“Studies of Iron Oxides, Ancient but Still Developing Family of Materials”

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Osaka University
“Synthesis and Characterization of Discrete Sandwich Com-
pounds Containing Palladium Chains or Sheets”

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National University of Singapore
“Our Attempts at Connecting Organometallic Clusters with
Nanoscience and Biology”

Dr TAKAO, Toshiro
Tokyo Institute of Technology
“Coupling Reaction of Pyridines Catalyzed by Di- and Trinuclear
Ruthenium Clusters”

Assoc Prof OKAZAKI, Masaaki
Kyoto University
“Introduction of Functional Groups onto the Fe₄C₄ Clusters”

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Institute for Molecular Science
“Early Transition Metal Complexes Bearing Phenoxide Multi-
dentate Ligands”

Prof XI, Zhenfeng
Peking University
“Development of Bimetallic Reagents for Organic Synthesis”

Dr NISHIURA, Masayoshi
RIKEN
“Reactivity of Metal-Carbon Bond in Metal-Carborane and
Metal-Carbonyne Complexes”

Prof XIE, Zuowei
The Chinese University of Hong Kong
“Reactivity of Metal-Carbon Bond in Metal-Carborane and
Metal-Carbonyne Complexes”

Assoc Prof ICHINOHE, Masaaki
University of Tsukuba
“Synthesis, Structure, and Reactivity of Stable Disilyne”

Assoc Prof OHSHIMA, Takashi
Osaka University
“Development of New Direct Catalytic Reactions Using Metal
Cluster Complexes”

Assoc Prof OGASAWARA, Masamichi
Hokkaido University
“Catalytic Asymmetric Synthesis of Planar-Chiral Metallocenes”

Assoc Prof LEE, Bun Yeoul
Ajou University
“Bimetallic Catalysis for Polymer Synthesis”

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Organized by Education and Research Organization for Genome
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17 December 2006 (Yokohama, Japan)

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Boston University, USA
“Large-scale Full-genome Comparisons: 40 Million Years of
Chromosome Inversions”

Prof JONES, David
University College London, UK
“Progress in Predicting Protein Folds and Protein-protein Inter-
actions from Amino Acid Sequence”

Prof WONG, Limsoon
National University of Singapore
“Exciting the Reluctant Bioinformatician”

Prof BLOMBERG, Anders
Göteborg University, Sweden
“To Bridge the Gap between the Theoretical and Experimental
Worlds - the Swedish National Research School in Genomics
and Bioinformatics”

Dr EBENHÖH, Oliver
Humboldt University Berlin, Germany
“Combining Education in Systems Biology and Bioinformatics”
(In place of the late Prof HEINRICH, Reinhart)

Prof KANEHISA, Minoru
Kyoto University and University of Tokyo
“Bioinformatics Education Integrating Basic Sciences and Prac-
tical Applications”

A decorative graphic consisting of two horizontal lines and two vertical lines. The top horizontal line is on the left, and the bottom horizontal line is on the right. A vertical line extends upwards from the left end of the top horizontal line, and another vertical line extends downwards from the right end of the bottom horizontal line. Small black squares are placed at the intersection of the top horizontal line and its vertical line, and at the intersection of the bottom horizontal line and its vertical line.

INDEX

NAME INDEX

[A]					
ABE, Katsumasa	34	HASEGAWA, Atsuko	22	ISOJIMA, Seiichi	48
AI NOI, Sauvaphap	34	HASHIDA, Masaki	46	ITO, Shingo	52
AKAI, Wataru	36	HASHIMOTO, Kosuke	60	ITO, Yoshiaki	50
AKI, Shiori	24	HASHISAKA, Masayuki	18	ITO, Yuichi	58
AKUTSU, Tatsuya	62	HATA, Yasuo	50	ITOH, Hiroyuki	44
AOYAMA, Takashi	24	HATAKEYAMA, Takuji	52, 79	ITOH, Masumi	60
ARITA, Toshihiko	12	HATTORI, Masahiro	60	IWAMOTO, Tatsuya	38
ASAMI, Koji	40	HAYASHI, Akito	56	IWASHIGE, Tomohito	38
AZUMA, Masaki	10	HAYASHI, Kazuhiro	8	IWASHITA, Yoshihisa	44
		HAYASHI, Kyohei	56	IWATA, Daiki	28
		HAYASHI, Yuji	36		
		HAYASHIDA, Morihiko	62	[J]	
[B]		HAYES, Nelson	60	JENSEN, Rader S	56
BROWN, John	62	HIDESE, Ryota	34	JIA, Yinggang	28
		HIGUCHI, Shinya	58	JITSUMORI, Keiji	34
[C]		HIMENO, Atsushi	18, 78, 81	JIU, Jinting	48
CHIBA, Yasuhiro	48	HIRABAYASHI, Tetsuo	36		
CHO, Jeong-Yong	22	HIRAI, Asako	28	[K]	
CHO, Uncho	62	HIRAI, Norihiko	12	KAI, Kosuke	22
CHUANG, Shih-Ching	6	HIRAKAWA, Mika	60	KAJI, Hironori	28
		HIRAMATSU, Takaaki	40	KAJITA, Kishiko	26
[D]		HIRANO, Daisuke	58	KAMISUKI, Shinji	26
DELMO, Michael Picazo	18	HIRANO, Toshiko	4	KAMIYAMA, Akane	22
DEMÉ, Bruno	71	HIRATA, Takafumi	30	KAN, Daisuke	10
DINH, Thi Thanh Hai	8	HIRATAKE, Jun	22	KAN, Keizo	8
		HIRONAKA, Koji	4	KANAYA, Toshiji	36
[E]		HIRORI, Hideki	58	KANEHISA, Minoru	60
ECHIZENYA, Yuki	36	HIROSE, Hisaaki	20	KANEMITSU, Yoshihiko	58, 79
EGUCHI, Yukihiko	70	HONDA, Wataru	60	KANIE, Yasumasa	28
ESAKI, Nobuyoshi	34	HORI, Akimi	4	KARAI, Yuki	36
		HORII, Fumitaka	28	KASAI, Naoko	10
[F]		HORITA, Junko	22	KASAI, Shinya	18, 78
FADIL, Hicham	79	HORIUCHI, Daisuke	54	KASHIMA, Hisashi	62
FUJII, Tomomi	50	HOSOKI, Koshin	58	KATAYAMA, Hiroyuki	56
FUJIMOTO, Shinji	44	HUANG, Jian	60	KATO, Hiroaki	22
FUJISAWA, Hiroshi	44	HWANG, Harold Y	70	KATO, Keisuke	6
FUJITA, Masashi	60			KATO, Utako	42
FUJITA, Michiyo	34	[I]		KATOH, Keiichi	40
FUKATANI, Yoshimi	22	ICHIHARA, Hisako	66	KAWABATA, Takeo	8, 80
FUKUDA, Masaaki	16	ICHII, Tomonori	38	KAWAI, Masahiro	4
FUKUDA, Takeshi	12, 74	CHIKAWA, Masahiro	44	KAWAI, Masanori	10
FUKUYAMA, Sadanobu	34	IDE, Kohei	22	KAWAI, Takahiko	36
FURUKAWA, Yukio	4	IKEDA, Yasunori	10	KAWAMOTO, Jun	34, 81
FUTAKI, Shiroh	20	IKEGAMI, Masahiro	44	KAWAMURA, Naohiro	22
		IKEUCHI, Hideyuki	22	KAWANISHI, Yutaka	38
[G]		IMAI, Kumiko	24	KAWASAKI, Rie	26
GAMO, Toshitaka	70	IMANISHI, Miki	20	KAWAZOE, Yoshinori	26
GAO, Weiping	12	INADA, Keiko	30	KAYAHARA, Eiichi	14
GHORAI, Sujit	52	INADOME, Hironori	42	KAYAMA, Yuzo	12
GIORDANI, Cristiano	32	INAGAKI, Hiroshi	82	KINOSHITA, Tomoko	32
GODA, Yuko	50	INAMURA, Koji	4	KISHIDA, Akio	70
GOTO, Atsushi	12	INOUE, Rintaro	36	KITA, Yasuo	40
GOTO, Shuichi	34	INOUE, Tadashi	38	KITAGAWA, Toshikazu	6
GOTO, Susumu	60	INOUE, Tadashi	58	KITAYAMA, Kaori	34
GUTTERIDGE, Alexander	60	INOUE, Takanori	18	KIYOMURA, Tsutomu	48
		INOUE, Hideyuki	58	KOBAYASHI, Kensuke	18
[H]		ISEKI, Toru	36	KOBAYASHI, Megumi	4
HAMADA, Yusuke	60	ISHIKAWA, Takehiro	44	KOBAYASHI, Sachiko	20
HAMAKI, Hirofumi	4	ISOBE, Toru	4	KOBAYASHI, Takeshi	20
HAMANO, Tsubasa	14	ISODA, Seiji	48	KOBAYASHI, Yu	14
HAMASAKI, Maho	42	ISODA, Yuka	42	KOHDA, Genki	56
HAN, Li-You	22				

KOJIMA, Kenji	60	MORIE, Jun	40	OKUDA, Shujiro	60
KOMATSU, Hiroshi	10	MORIGUCHI, Sakumi	48	OMI, Rie	34
KOMATSU, Koichi	6	MORINAGA, Takashi	12	OMI, Yohei	12
KOMATSU, Shigeo	52	MORISAKI, Tatsuya	20	OMORI, Taketo	34
KONDO, Jun	50	MORIYA, Yuki	60	ONO, Teruo	18
KONDO, Yoshiyuki	52	MORIYAMA, Katsuhiko	8, 80	ONUKE, Ritsuko	60
KONDOU, Kouta	18	MOROOKA, Saiko	32	OOTAKA, Ryu	62
KONO, Tomohiro	30	MOURI, Kazunari	62	ORIHARA, Tsubasa	26
KOSUGE, Michie	20	MUKAIHARA, Yoko	56	OZAKI, Shuhei	4
KOUNO, Ryo	16	MURACHI, Yuki	14	OZAWA, Fumiyuki	56
KOYAMA, Dai	34	MURAKAMI, Hiromi	56		
KOZAWA, Ryouhei	48	MURAMATSU, Wataru	8		
KUBO, Akira	42	MURATA, Michihisa	6, 77	[P]	
KUGA, Takako	28	MURATA, Yasujiro	6, 77	POOLSAP, Unyanee	62
KUGIMIYA, Akira	26	MURDEY, Richard James	40		
KUMA, Kei-ichi	66	MUTO, Ai	60	[Q]	
KUMADA, Nobuhiro	54	MUTOH, Yuichiro	56	QIAO, Xiuying	38
KUNYOSHI, Minoru	16			QU, Li-Jia	24
KURAHASHI, Kensuke	30	[N]			
KURAMOTO, Mamoru	12	NACHER, Jose C	62	[R]	
KURATA, Chizu	22	NAGAHORA, Noriyoshi	4, 77	RAHMAN, Nelly	36
KURATA, Hiroki	48	NAKAGAWA, Shuko	24	RUIZ, Diego Deiz	60
KURIHARA, Tatsuo	34	NAKAGAWA, Yuichi	22		
KURITA, Naoyoshi	32	NAKAGAWA, Yusuke	30	[S]	
KUROKAWA, Suguru	34	NAKAHARA, Masaru	32	SAINO, Hiromichi	22
KUROTOBI, Kei	6	NAKAJIMA, Risa	26	SAITO, Takashi	54
KUSAKA, Masashi	28	NAKAMURA, Atsushi	20	SAKABE, Shuji	46
KUSANO, Hiroaki	24	NAKAMURA, Kaoru	4, 80	SAKAI, Daisuke	62
KUSUDA, Toshiyuki	18	NAKAMURA, Kinu	24	SAKAI, Hiroki	60
KUWAMOTO, Kiyoshi	48	NAKAMURA, Masaharu	52, 79	SAKAI, Maiko	10
		NAKAMURA, Shu	44	SAKAKURA, Shusuke	50
[L]		NAKAMURA, Shuji	18	SAKATA, Kanzo	22, 75
LADMIRAL, Vincent	12	NAKAMURA, Yasunori	20	SAKIYAMA, Tadahiko	60
LEONG, Weng Kee	71	NAKANISHI, Tsutomu	70	SASAKI, Yoshihiro	30
LI, Linchuan	24	NAKAO, Masao	44	SASAMORI, Takahiro	4, 77
LI, Yuan-Hui	30	NAKASE, Ikuhiko	20, 78	SASAMURA, Tatsuya	40
LIMVIPHUVADH, Vachiranee	60	NAKATA, Kunihiko	16	SASE, Shohei	52
LIU, Jingjing	24	NAKATSUJI, Ryo	38	SATO, Ayato	26
LUO, Qing	28	NAKATSUKA, Seiji	30	SATO, Naoki	40
		NEMOTO, Takashi	48	SATO, Tetsuya	66
[M]		NISHIDA, Koji	36	SAWADA, Toshiaki	38
MA, Ying	12	NISHIJIMA, Yoshihito	34	SENOO, Kazunobu	14
MAMITSUKA, Hiroshi	64	NISHIKAWA, Mayumi	32	SESEI, Takashi	28
MASUNO, Shinichiro	46	NISHIKAWA, Miwako	42	SETO, Mari	48
MATSUBA, Go	36	NISHIMURA, Kousuke	10	SHIBATA, Takeshi	8
MATSUDA, Kazunari	58, 80	NISHIYAMA, Gen-ichiro	34	SHIGA, Motoki	64
MATSUDA, Kazuomi	16	NODA, Akira	44	SHIGAKI, Yuta	34
MATSUDA, Seiji	8	NOMURA, Akihiro	12	SHIGEMIZU, Daichi	60
MATSUMIYA, Yumi	38	NORISUYE, Kazuhiro	30	SHIMAKAWA, Yuichi	10
MATSUMOTO, Atsushi	14	NOSHIRO, Daisuke	20	SHIMIZU, Akiyoshi	30
MATSUMOTO, Takeshi	4			SHIMIZU, Bun-ichi	22
MATSUMOTO, Teruyuki	4, 80	[O]		SHIMIZU, Yugo	60
MATSUNAGA, Ryusuke	58	OCHI, Yuta	6	SHIMOGAWA, Hiroki	26
MATUBAYASI, Nobuyuki	32, 79	OGAWA, Ai	50	SHINOHARA, Tokuyuki	26
MIHARA, Hisaaki	34	OGAWA, Hiroki	36	SHINTAKU, Hiroki	44
MIKAWA, Kohei	32	OGAWA, Tetsuya	48	SHIRAI, Toshiyuki	44
MINAMI, Tomoharu	30	OH, Min-A	60	SHIRAKI, Hiroshi	10
MINO, Akira	28	OHMINE, Kyoko	28	SHISHIOH, Nobue	42
MISHIMA, Eri	14	OHNISHI, Toshiyuki	22, 81	SOHRIN, Yoshiki	30
MIYAKAWA, Yuya	16	OHNO, Kohji	12, 77	SOUDA, Hikaru	44
MIYAKE, Ryoma	34	OISHI, Yohei	38	SUE, Daisuke	8, 80
MIYAZAKI, Akira	26	OKA, Atsuhiko	24	SUGA, Akitsugu	60
MIZOTA, Hirohisa	50	OKA, Kengo	54	SUGISAKI, Hiroyuki	24
MIZUHATA, Yoshiyuki	4, 77	OKA, Takahiro	8	SUGIYAMA, Yusuke	4
MIZUTANI, Masaharu	22, 78	OKA, Takanori	16	SUZUKI, Masaru	16
MOCHAMAD, Lutfi Firdaus	30	OKADA, Shinichi	38	SUZUKI, Shinji	28
MOHAMMED, Amr Hassan	34	OKAMURA, Emiko	32		
MONGUCHI, Daiki	8	OKAYASU, Kenji	12	[T]	
MORI, Sadayuki	6	OKAZAKI, Masaaki	56	TABATA, Hiroshi	12

TADOKORO, Akiko	20	UEDA, Nobuhisa	62	[Z]	
TAI, Liz	22	UEMURA, Kouji	16	ZHANG, Wanjiao	34
TAI, Yugo	12	UESUGI, Motonari	26, 78	ZHU, Shanfeng	64
TAJIMA, Hiroyuki	71	UMEDA, Masato	42	ZOU, Yanhui	50
TAJIMA, Yujiro	44	UMETANI, Shigeo	30		
TAKADA, Yuko	56	URABE, Shinji	44		
TAKAGI, Junpei	26	URATA, Takashi	62		
TAKAHARA, Keigo	42	URUNO, Yoshiharu	8		
TAKAHASHI, Masahide	16	URUSHIHARA, Shohei	30		
TAKAHASHI, Ryosuke	14	USAMI, Akiko	14		
TAKAISHI, Kazuto	8	UTSUNOMIYA, Machiko	34		
TAKANO, Masato	56	UYAMA, Makoto	8		
TAKANO, Mikio	54, 76				
TAKARABE, Masataka	60	[V]			
TAKAYAMA, Kentaro	20	VALLURU, Reddy Krishna	8		
TAKEDA, Nobuhiro	4				
TAKEDA, Taijiro	36	[W]			
TAKEMOTO, Kazuhiro	62	WAKAI, Chihiro	32		
TAKEMURA, Kazunobu	14	WAKATA, Tsutomu	12		
TAKEUCHI, Ken-ichi	42	WAKIOKA, Masayuki	56		
TAKEUCHI, Kosaku	4	WAN, Raymond	64		
TAKEUCHI, Shigeki	62	WANG, Jianyi	32		
TAKEUCHI, Toshihide	20	WARNICKE, Peter	18		
TAKEUCHI, Yoshinori	22	WATANABE, Hiroshi	38		
TAKIGAWA, Ichigaku	64	WATANABE, Toshihide	8		
TAMADA, Yoshinori	18				
TAMURA, Takeyuki	62	[Y]			
TANABE, Fumiyuki	6	YAJI, Toyonari	48		
TANABE, Mikio	44	YAMADA, Ikuya	54		
TANABE, Taro	4	YAMADA, Keisuke	18		
TANAKA, Michihiro	60	YAMADA, Takeshi	14		
TANAKA, Nobutoshi	34	YAMADA, Takuji	60		
TANAKA, Nobuya	60	YAMADA, Tomonori	28		
TANAKA, Yumi	34	YAMADA, Yoichi	71		
TANAKA, Yusuke	16	YAMAGO, Shigeru	14		
TANIGAWA, Hironobu	18	YAMAGUCHI, Koji	22		
TANIGUCHI, Masatoshi	24	YAMAGUCHI, Yukiko	42		
TANIGUCHI, Yukimi	24	YAMAMOTO, Hideaki	16		
TANIMA, Daisuke	8	YAMAMOTO, Junpei	36		
TANIUCHI, Kentaro	42	YAMAMOTO, Kentaro	34		
TERADA, Tomoko	8	YAMAMOTO, Ryotaro	22		
TERAOKA, Fumiteru	8	YAMAMOTO, Shinpei	54, 79		
TERUI, Daisuke	30	YAMAMOTO, Yasutaka	56		
TEZUKA, Miho	12	YAMANE, Hiroaki	52		
TOBE, Ryuta	34	YAMANISHI, Yoshihiro	60		
TOCHIO, Tatsunori	50	YAMAUCHI, Takae	34		
TOGAI, Manabu	14	YAMAZAKI, Daisuke	6		
TOHNO, Shunsuke	20	YAMAZAKI, Eriko	42		
TOKITA, Shigeki	46	YAN, Wei	20		
TOKITOH, Norihiro	4	YANG, Hu	28		
TOKUDA, Yomei	16	YANO, Kuniaki	18		
TOMA, Gabriel	52	YASAKA, Yoshiro	32		
TOMOHISA, Hiroshi	36	YASUDA, Hideki	58		
TOMOTO, Hiroo	22	YASUDA, Keiko	24		
TONGU, Hiromu	44	YASUKAWA, Go	22		
TORAYA, Terumasa	34	YOKO, Toshinobu	16		
TOSAKA, Masatoshi	14	YOKOYAMA, Izumi	34		
TSUBAKI, Kazunori	8	YOSHIDA, Hiroyuki	40		
TSUCHIDA, Akira	60	YOSHIDA, Kaname	48		
TSUGE, Tomohiko	24, 78	YOSHIDA, Ken	32		
TSUJI, Masaki	14	YOSHIDA, Ryohei	6		
TSUJII, Yoshinobu	12	YOSHIKAWA, Chiaki	12, 81		
TSUJIMOTO, Masahiko	48	YOSHIMURA, Ken-ichi	56		
TSUMOTO, Kouhei	71	YOSHIMURA, Tomoyuki	8		
TSURUSAKI, Akihiro	4	YOSHIOKA, Taiyo	14		
TSUTSUMI, Jun'ya	40	YOSHIOKA, Yu	12		
		YOSHITOMI, Takahiko	56		
[U]		YOSHIKAWA, Akiyasu	60		
UCHIDA, Hirohito	36	YUASA, Akihiro	4		

KEYWORD INDEX

[A]		[G]		Nano-Fabrication	18
Amino Acid Metabolism	34	Gel Filtration Analysis	50	Nano Molecular Hybrids	28
Aromaticity	6	Generation of High Energy Radiation	46	Nanoparticle	54
Artificial Multilayers	18	Genome	60	Nano-Structure Formation	46
Asymmetric Synthesis	8	Glass Structure	16	Near-Field Scanning Optical Microscopy	58
[B]		Glycosidase	22	NMR	32
Bacterial Cellulose	28	Glycosylation	14	Nucleophilic Catalysis	8
Behavior	42	Graph Algorithms	62	[O]	
Biogeochemistry	30	[H]		Oligonaphthalene	8
Bioinformatics	60, 64	Halogen Biochemistry	34	Oligosaccharide Synthesis	14
[C]		H/D Exchange	32	Open-Cage Fullerene	6
Carbon-Carbon Bond Formation	52	Heteroatom	4	Organic EL Materials	28
Cell Differentiation	24	Heteroatom Chemistry	14	Organic-Inorganic Hybrid Material	16
Cell Division	24	Hierarchic Structure	36	Organo Main Group Metal Reagent	52
Cell Morphogenesis	42	High Pressure Synthesis	54	[P]	
Charge Selectivity	40	Highly Amphoteric Polar Molecule	40	Pathway Analysis	60
Chemical Biology	26	Highly Organized Materials	28	Peptide Design	20
Chemical Genetics	26	Homogeneous Catalyst	56	Phase Rotation	44
Chemical Genomics	60	[I]		Phenylpropanoid	22
Chemical Library	26	I ^c	50	Photoactive Material	16
Chemoinformatics	62	Inhibitor	50	Phylogenetic Tree	66
Cold-Adapted Microorganism	34	In-situ Small Angle X-ray Scattering Measurement	36	Polymer Thin Film	36
Colloidal Crystal	12	Intracellular Delivery	20	Polymorphic Phase Transition	40
Computational Biology	64	Ion Channel	40	Polyploidy	24
Concentrated Polymer Brush	12	Ionic Liquid	32	Precise Structure Analysis	10
π -Conjugated Systems	6	Iron Catalyst	52	Protein-Protein Interaction	66
Coulomb Explosion	46	[K]		[Q]	
CPY	50	KEGG	60	Quantum Transport	18
Crystal Structure	50	Kernel Methods	62	Quorum Sensing	66
Crystallization under Shear Flow	36	Kinetic Stabilization	4	[R]	
Cyclin	24	[L]		Radical Reaction	14
Cytochrome P450	22	Laser Cooling	44	Reaction Mechanism	56
[D]		Laser Produced Ion	44	Rheology	38
Data Mining	64	Lipid Metabolism	42	Rheo-Optics	38
Dewetting and Phase Separation	36	Living Radical Polymerization	12, 14	[S]	
Dielectric Spectroscopy	38	Low-Coordinated Species	4	Scale-Free Networks	62
DNA Binding Protein	20	Low-Melting Glass	16	Scanning Probe Microscopy	48
Dynamic Chirality	8	[M]		Selenium Biochemistry	34
[E]		Machine Learning	64	Semiconductor Nanoparticles	58
Electric Birefringence	38	Magnetic Ferroelectrics	10	Small Molecules	26
Electron Beam Cooling	44	Magnetic Materials	18	Solid-Phase Extraction-ICP-MS	30
Electron Microscopy	48	Magnetism	54	Solid-State NMR	28
Endohedral Fullerene	6	Marine Chemistry	30	Spintronics	18
Endoreduplication	24	Membrane Lipid	42	Steric Protection	4
Energetic Ion Generation	46	Membrane-Permeable Peptides	20	Strong Permanent Magnet	44
Enzyme Mechanism	22	Metal-insulator Transition	10	Substitution Reaction	52
Epitaxial Thin Films	10	Micro/Nano Structure Fabrication	16	Sulfur Biochemistry	34
[F]		Molecular Evolution	66	Surface Grafting	12
Femtosecond Laser Spectroscopy	58	Molecular Recognition	8	Synergistic Effect	56
FET	48	Molecular Stacking Column	40	Synthetic Organic Reaction	52
Fine Particle	12	Multiple Alignment	66	Systems Biology	62, 64
Formic Acid	32	[N]		[T]	
Fullereryl Cation	6	Nanodiffraction	48	Thermoregulation	42
Functional Transition Metal Oxides	10	[O]		Thin Layer Fabrication	54

Titanate Nanotube	48
Trace Metals	30
Transition Metal Clusters	56
Transition Metal Complex	56
Transition Metal Complexes	4
Transition Metal Oxides	54
Transition-State Analog Inhibitors	22
[W]	
Water-Gas-Shift Reaction	32
Western North Pacific	30
[Z]	
Zinc Finger Peptide	20