

# ICR ANNUAL REPORT 2003 (Volume 10) - ISSN 1342-0321 -

For the calendar year 1 January 2003 to 31 December 2003

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# Published and distributed by:

Institute for Chemical Research (ICR), Kyoto University

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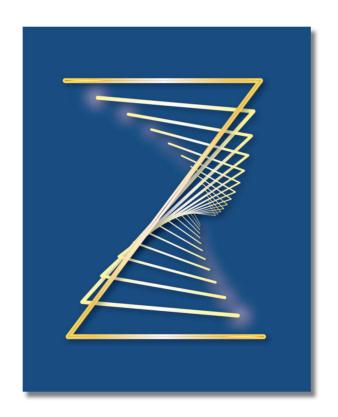
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URL http://www.kuicr.kyoto-u.ac.jp/index.html

### Printed by

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Ogawa Higashi-iru, Shimodachiuri, Kamigyo-ku, Kyoto 602-8048, Japan.
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# ICR ANNUAL REPORT 2003



Institute for Chemical Research Kyoto University

Volume 10

# Preface



It is a great pleasure for us to publish the ICR Annual Report for 2003.

In April 2003 a new research center named "International Research Center for Elements Science" has started. This center consists of four laboratories and two guest laboratories and covers the fields of organic synthesis, inorganic synthesis, coordination chemistry, and photoquantum nanochemistry.

We have appointed seven new full professors, Professor UMEMURA Junzo for the Laboratory of Solutions and Interfaces (appointed in June), Professor SHIMAKAWA Yuichi for the Laboratory of Advanced Inorganic Synthesis (October), Professor UMEDA Masato for the Laboratory of Biopolymer Structure (February), Professor OZAWA Fumiyuki for the Laboratory of Organotransition Metal Chemistry (September), Professor SAKABE Shuji for the Laboratory of Beams and Fundamental Reaction (April), Professor MATSUKI Seishi for the same laboratory (June), and Professor KANEMITSU Yoshihiko for the Laboratory of Photonic Elements Science (January 1, 2004).

Thus ICR has been expanded to a system of 9 divisions and 3 affiliated research centers in April 2003, consisting of 31 laboratories and 6 guest-laboratories. At the present time, 29 full professors, 23 associate professors, 40 instructors, 5 guest professors, and 6 guest associate professors work in the ICR, and about 210 graduate students and approximately 40 foreign researchers study at the ICR.

A new Kyoto University 21st Century COE Program entitled "Knowledge Information Infrastructure for Genome Science" was initiated as a joint venture between the Bioinformatics Center of the ICR and the School of Pharmaceutical Sciences. The program lead by Prof. KANEHISA of our Institute aims at establishing the knowledge information infrastructure for the 21st century genome science, both in terms of the computerized resource and the human resource. A

new education/training program is being introduced, integrating traditional bioinformatics with physics and chemistry and with medical and pharmaceutical sciences.

Another Kyoto University 21st Century COE Program named 'Center for Diversity and Universality in Physics' started in July. In this program Department of Physics and Department of Astronomy of Graduate School of Science, Yukawa Institute for Theoretical Physics, Kwasan and Hida Observatories, International Innovation Center, and the ICR are involved. Intended through this program is the establishment of an outstanding activity center for research and education on fundamental physics and astrophysics, covering elementary particles and nuclei, atoms and molecules, macroscopic systems including life, celestial objects, and the largest system: the universe.

The organization of national universities must and will be significantly changed by transformation into independent administrative corporations in April of 2004. With this goal in mind, we understand that we must work together in order to keep and strengthen the vitality of our Institute, while overcoming the inevitable turning points and changes which lie ahead. To be successful, we must provide strong support and leadership in all areas of our research activities for the development of science and technology. For this purpose, we will continue to devote our efforts to fundamental research and its application in specific fields which are important to our future well being, health and prosperity.

Meso Taband

January 2004

Mikio Takano Director

# ICR News 2003

# The Establishment of "International Research Center for Elements Science"



■ Director of IRCELS: Prof TAMAO, Kohei

The "International Research Center for Elements Science" (IRCELS) as our new attached research center has started its activity from April 1, 2003.

On January 9, 2004, our Institute celebrated the opening of this new center IRCELS by performing the commemorative ceremony at the seminar hall, in the presence of Professor Kazuo Oike, President of Kyoto University, Mr. Yoshiyuki Satoh, Deputy Director (Research Institutes Cooperation) of the Research Promotion Bureau of Ministry of Education, Culture, Sports, Science and Technology (MEXT: Monbukagaku-sho), and Professor Mitsuhiko Araki, Dean of the Graduate School of Engineering, who delivered the congratulatory addresses. Our Director, Professor Mikio Takano, gave the opening and thanking remarks. Finally, Tamao, Director of IRCELS, introduced the organization and staff of the new Center.



President Oike said, "In the tripartite structure of three campuses of Kyoto University, the Uji Campus is regarded as the basis for advanced science and technology research. The development of advanced science of Uji Campus, where the top-class research institutes and centers of natural sciences are clustered, is considered as one of the most important issues."





The opening ceremony was held as the morning session of the 3rd International Symposium of Kyoto COE Project "Elements Science". In the Commemoration Session, three Plenary lectures were given by the distinguished guests, Prof. Koji Kaya, Director of Institute for Molecular Science, and two foreign guests.

http://www.kuicr.kyoto-u.ac.jp/IRCELS/index\_e.html

# A New 21st Century COE Program "Center of Research and Knowledge Information Infrastructure for Genome Science"



Project Leader: Prof KANEHISA, Minoru
(Director of Bioinformatics Center)

A grand challenge in the genome science of the 21st century is to computationally predict systemic functional behaviors of the cell, the organism, and the biosphere from genomic and molecular information, especially for the purpose of medical, industrial, and other practical applications. This will require new bioinformatics, not simply for screening large-scale data, but rather for reconstructing the system and computing its interactions with the environment.

The 21st Century COE program "Genome Science", a joint venture between the Bioinformatics Center of the Institute for Chemical Research and the School of Pharmaceutical Sciences in Kyoto University, aims at establishing the knowledge information infrastructure for the 21st century genome science, both in terms of the computerized resource and the human resource. A new education/training program is being introduced, integrating traditional bioinformatics with physics and chemistry and with medical and pharmaceutical sciences.





A symposium celebrating the inauguration of the 21st Century COE program was held at the Sakagura VIL (Venture-business Incubation Laboratory) on August 8, 2003.

This COE program was adopted on July 21, 2003.

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

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# - ${f A}$ bbreviations used in the columns

Prof Em	Professor Emeritus	Res	Researcher
Prof	Professor	A Res	Assistant Researcher
Vis Prof	Visiting Professor	RF	Research Fellow
Assoc Prof	Associate Professor	RS	Research Student
Vis Assoc Prof	Visiting Associate Professor	GS	Graduate Student
Lect	Lecturer	DC	Doctoral Course (Program)
Lect(pt)	Lecturer (part-time)	MC	Master's Course (Program)
Instr	Instructor	UG	Undergraduate Student
Vis Instr	Visiting Instructor	D Sc	Doctor of Science
Assoc Instr	Associate Instructor	D Eng	Doctor of Engineering
Techn	Technician	D Agr	Doctor of Agricultural Science
Guest Scholar	Guest Scholar	D Pharm Sc	Doctor of Pharmaceutical Science
Guest Res Assoc	Guest Research Associate	D Med Sc	Doctor of Medical Science
PD	Post-Doctoral Research Fellow	Ph D	Doctor of Philosophy
	1		

# TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Key to headline in the columns

\* See also "ORGANIZATION AND STAFF" on pages 114 and 115.

# **States and Structures**- Atomic and Molecular Physics -

# http://elec.kuicr.kyoto-u.ac.jp



Prof HATA, Yasuo (D Sc)



Assoc Prof ITO, Yoshiaki (D Sc)



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Instr FUJII, Tomomi (D Sc)



A Res TOCHIO, Tatsunori (D Sc)

# **Students**

OoHASHI, Hirofumi (D3) HAYASHIDA, Minoru (D3) SAKAKURA, Shusuke (M1) MIZOTA, Hirohisa (M1)

# **Visitors**

Prof FRICKE, Burkhard Dr SHARMA, Sangeeta University of Kassel, Germany, 10-11 March 2003 Institute of Theoretical Physics, University of Graz, Austria, 8-18 September 2003

# Scope of Research

The research activities in this laboratory are performed for X-ray structural analyses of biological macromolecules and inorganic 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 structural analyses of inorganic materials, the electronic states of atoms and molecules are investigated in detail using conventional X-ray and SR in order to obtain fundamental information on the property and structure of materials. The theoretical analysis of the electronic states and the development of new radiation detectors are also performed.

# Research Activities (Year 2003)

# **Presentations**

Crystallographic analyses of enzyme functions in the field of agricultural chemistry; Hata Y, Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 3 April.

Similarities between protein-protein and protein-carbohydrate interactions of pokeweed lectins; Hayashida M, Fujii T, Ishiguro M (Kyushu), Hata Y, Annual Meeting, Prot. Sci. Soc. Jpn., 25 June.

Crystal structure of thermostable aspartase and structure-based exploration of functional sites in the aspartase family; Hata Y, Fujii T, Sakai H, Kawata Y (Tottori), Broome2003 Int. Crystallography Meetings AsCA'03/Crystal-23, 12 August.

*K*α x-ray emission spectra of Cr compounds; Tochio T, Ito Y, Sherman E Y, Ambrosch-Draxl C, Vlaicu A M, Fukushima S, Shoji T, Nineth Wien-Workshop, Vienna, Austria, April 23-26, 2003.

# **Grants**

Hata Y, Protein-engineering studies on the unique conformations and the expression mechanism of function of pokeweed lectines, Grant-in-Aid for Scientific Research on Priority Areas (C) (2), 1 April 2002 - 31 March 2004.

Hata Y, Structural analyses of gene-products involved in protein structure formation, Protein 3000 Project, 1 April 2002 - 31 March 2007.

Fujii T, Elucidation of mechanism of structural change in functional sites of aspartase, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.

# X-ray crystal structure analysis of pokeweed lectin PL-C

Pokeweed lectin (PL) is a mitogenic lectin, which is specific for *N*-acetylglucosamine-containing saccharides and exceptionally activates both T and B cells. Five lectins, designated PL-A, PL-B, PL-C, PL-D1, and PL-D2, have been isolated from the roots of pokeweed. PL-C is a mitogen but exhibits no heamagglutinating activity. The polypeptide chain of PL-C consists of three chitin-binding domains, each of which has four S-S bridges and the putative saccharide-binding site.

The crystal structure of PL-C has been solved by the isomorphous replacement method and refined up to 1.8 Å resolution with the *R*-factor of 17.6%. Two subunits in the asymmetric unit of the PL-C crystal are related to each other by the non-crystallographic 2-fold axis and form a dimer in a head-to-tail fashion with three pairs of putative carbohydrate-binding sites facing each other (Figure 1). All the sites in the subunit are located in the dimer interface. The dimerization of PL-C is performed through the hydrophobic interactions between the putative carbohydrate-binding sites of opposite domains in the dimer. The PL-C dimer has no room for accommodating the carbohydrate. Therefore, the loss of carbohydrate-binding ability due to self-association probably the reason that PL-C exhibits no agglutinating activity.

# Domain-III Domain-III' Domain-III Domain-III' Domain-III Domain-III' N' Domain-III Domain-III' N Domain-III Domain-III' Domain-III Domain-III'

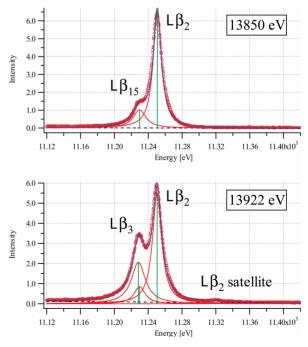
Figure 1. The PL-C dimer structure.

### Photon cooking

The third generation synchrotron radiation such as SPring-8 is very intense and tunable x-ray source, and offers detailed photoexcitation measurements around the threshold regions. Especially, X-ray emission spectroscopy is a suitable tool to study the satellites due to the electron correlation.

Pt  $L\beta_{15}$  ( $L_{III} \rightarrow N_{IV}$ ) emission line has not been yet confirmed due to the overlap of Pt  $L\beta_3$  ( $L_I \rightarrow M_{III}$ ) diagram line. However, the energy value of Pt  $L\beta_{15}$  emission can be obtained using a high resolution X-ray spectrometer with tunable photon energies around  $L_1$  threshold.

The incident photon energy was scanned in the energy range around the Pt  $L_1$  edge. Two excitation energies were used below and above the  $L_1$  edge (13880.7 eV). Pt  $L\beta_{15}$  emission line overlaps  $L\beta_3$  line above the edge, only Pt  $L\beta_{15}$  diagram line could finally be obtained below the edge as seen in figure 2. It took more than a half century to get this value.



**Figure 2.** Pt  $L\beta_{2,3,15}$  obtained below and above  $L_1$  edge

# **States and Structures** - Electron Microscopy and Crystal Chemistry -

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



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Visitor

Dr GLOTTER, Alexandre

Laboratoire de Physique des Solides, CNRS, France, 21-22 November 2003

# **Scope of Research**

Structures of materials and their structural transition associated with chemical reactions are studied through direct observation of atomic or molecular imaging by high-resolution spectromicroscopic method which realizes high resolution energy-filtered imaging as well as electron energy-loss spectroscopy. 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 with scanning probe microscopic methods, the following subjects are studied: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, fabrication of low-dimensional functional assemblies.

# Research Activities (Year 2003)

# **Presentations**

Replacement of Molecules at Liquid/Solid Interface, Takajo D, Nemoto T, Isoda S, Seminar of Nano-scale Science and Technology at Kyoto University, 31 January.

Organic Epitaxy at Gas/Solid and Liquid/Solid Interfaces, Nemoto T, Isoda S, 2nd International Conference on Molecular Electronics and Bioelectronics, 7 March.

Controlling Alignment of Phthalocyanine on Organic Mono-molecular Layer, Takajo D, Nemoto T, Isoda S, Workshop of Nano-scale Organic Dye, 28 March.

Grain Boundary Effect and Single Grain Property in Organic Field Effect Transistors, Minari T, Kyoto Univ. 21st Century COE, Rennes-Japan Meeting, 27 September.

Device Structures and Electrical Properties of CuPcF<sub>16</sub> Field Effect Transistor, Minari T, Fujiwara E(IMS), Takada M (GUAS), et al., Korea-Japan Joint Forum 2003, 29 September.

Characterization of Graetzel Dye on TiO<sub>2</sub> Particles by Transmission Electron Microscopy, Yoshioka Y, Tsujimoto M, Koshino M, et al., Korea-Japan Joint Forum 2003, 1 October.

Organization of Copper-phthalocyanine Molecules on Mono-molecular Organic Buffer Layers, Takajo D, Nemoto T, Ozaki H(TUAT), et al., 1st Int. Meeting Appl. Phys., 14 October.

Molecular-scale Structure Fabrication at Liquid/Solid

# Replacement of Molecules at Liquid/Solid Interface

Perylene-3,4,9,10-tetracarboxylic-dianhydride (PTC-DA) mono-molecular layer was formed onto a highly ordered pyrolytic graphite (HOPG) by vacuum-deposition. After 17,19-dotetracontadiyne (DTDY) in phenyloctane solution was dripped on the above sample, a tip of scanning tunneling microscope (STM) was inserted into the solution and scanned to scratch a part of mono-molecular layer of PTCDA from HOPG substrate. (Fig.1) DTDY molecules were observed to be adsorbed onto the scratched region of PTCDA molecular layer to form a mono-molecular layer. The orientation and size of DTDY molecular layer could be controlled by selecting the scanning direction and area of STM tip to scratch. This method is one of promising fabrications of nano-scale structure at liquid/solid interfaces.

1. Takajo D, Nemoto T, Kurata H, et al., Thin Solid Films, 438-439, 428-432 (2003).

# Inhomogeneous Substitution of Polyhalogenated Copperphthalocyanine Studied by High-resolution Imaging and Electron Crystallography

This study was aimed at distinguishing halogen atoms substituted in a molecule of copper-phthalocyanine (CuPc) by high-resolution transmission electron microscopy (HRTEM). The subject was carried out on octabromoctachloro-CuPc, and the obtained HRTEM images suggested inhomogeneous distribution of bromine and chlorine atoms at 1-, 2-, 3- and 4- substitution positions of CuPc in image contrast. (Fig.2) As a result of electron crystallography the occupancy of bromine atoms at the 1-position (and equally at the 4-position) was found to be 52%, which is slightly

Interfaces, Takajo D, Nemoto T, Isoda S, 1st Int. Meeting. Appl. Phys., 14 October.

Development of Nanotip FEG for STEM and ELNES Analysis, Kurata, H, International Workshop on High Resolution TEM and GIF Investigation of Nanomaterials, 12 December.

### **Grants**

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2003 - 31 March 2004.

Kurata H, Local State Analysis of Organic Materials by

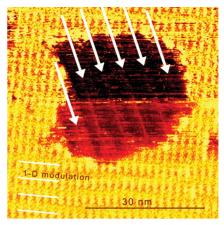


Fig. 1 STM image of PTCDA after scratching

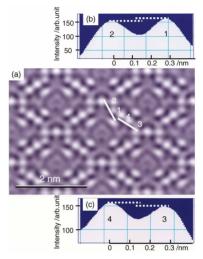


Fig. 2 HRTEM image of polyhalogenated CuPc.

higher than for random substitution. This small deviation causes apparent inhomogeneous image contrast of halogen substitution observed in the high-resolution images, as concluded from computer simulation of images. Such potential to detect inhomogeneity in substitution by TEM should be important for the chemical understanding of substitution reactions at the atomic level.

2. Kobayashi T, Ogawa T, Moriguchi S, et al., J. Electron Microsc., 52, 85-90 (2003)

Spatially and Angular Resolved EELS, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2006.

Ogawa T, Observation of the Production Process of Metal Nano-rod by Colloidal Method Using Cryo-TEM, Grant-in-Aid for Scientific Research, Promotive Research, 1 April 2003 - 31 March 2005.

### **Award**

Kurata H, The Japanese Society of Microscopy Award, Development of Electron Energy-loss Spectroscopy and Its Application to Local State Analysis of Materials, The Japanese Society of Microscopy, 8 June 2003.

# States and Structures - Polymer Condensed States -

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



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### Visitor

Dr COOK, Stuart The Tun Abdul Razak Research Centre, United Kingdom, 14 November 2003

# **Scope of Research**

Attempts have been made to elucidate the molecular arrangement and the mechanism of structural formation/change in crystalline polymer solids, polymer gels and elastomers, polymer liquid crystals, and polymer composites, mainly by electron microscopy and/or X-ray diffraction/scattering. The major subjects are: synthesis and structural analysis of polymer composite materials, preparation and characterization of polymer gels and elastomeric materials, structural analysis of crystalline polymer solids by direct observation at molecular level resolution, and in situ studies on structural formation/change in crystalline polymer solids.

# Research Activities (Year 2003)

# **Presentations**

TEM studies on thin films of natural rubber and polychloroprene crystallized under molecular orientation, Tsuji M, Shimizu T, Tosaka M, Kohjiya S, The 9th International Seminar on Elastomers (ISE 2003), Kyoto, 2 - 4 April and other 8 presentations.

Elastomeric branched poly(ethylene oxide) as a matrix for functionality materials, Kohjiya S, Ikeda Y, Meeting of the Rubber Division, American Chemical Society, Sanfrancisco, California, USA, 28 - 30 April.

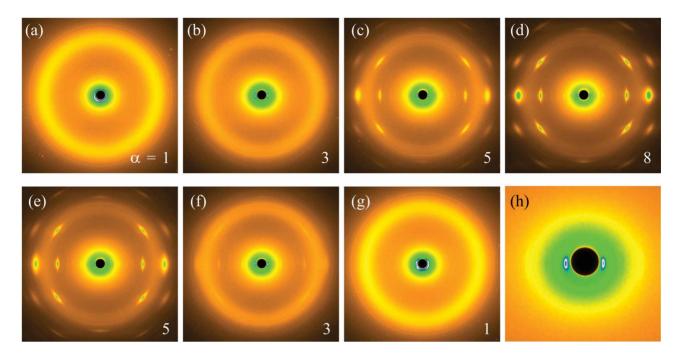
Crystallization of natural rubber during drawing as evaluated by synchrotron X-ray diffraction method - Relationship between structural development and mechanical properties -, Murakami S, Atsumi K, Senoo K, Kohjiya S, Kotera M, Toki S, Spring Meeting, The Society of Polymer Science, Japan, Nagoya, 28 - 30 May and other 5 presentations.

Morphological study by TEM on uniaxially oriented thin films of PET, PEN and their blends, Yoshioka T, Tsuji M, Kawahara Y, Kohjiya S, Polymer Processing Society (PPS-19), Melbourne, Australia, 7-10 July.

Novel polymer electrolytes based on branched poly(oxyethylene) and inorganic sulfide glass, Kohjiya S, European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2003), Lausanne, Switzerland, 1 - 5 September.

Reinforcing effect of silica generated in situ on general purpose grade rubbers, Kohjiya S, Ikeda Y, Euro Fillers 2003, Alicante, Spain, 8 - 11 September.

Strain-induced crystallization and physical properties of natural rubber, Kohjiya S, Tosaka M, Murakami S, Poompradub S, Ikeda Y, Toki S, Sics I, Hsiao B, Autumn Meeting, The Society of Polymer Science, Japan, Yamaguchi,



**Figure 1.** Sequential change of WAXD patterns from NR-4. Stretching direction is vertical. Corresponding strain values are indicated at the right bottom in parts (a) to (g) of the figure. Part (h) shows the enlarged image of the center of part (b). Sharp reflections from fatty acids are recognized on both sides of the beamstop (s = 0.24).

# Orientation and crystallization of natural rubber network as revealed by WAXD using synchrotron radiation

Strain-induced crystallization of natural rubber samples with various network-chain densities, n, was investigated by synchrotron X-ray diffraction measurements. It was found that the onset strain of crystallization was almost independent of n. Lateral crystallite size and degree of orientational fluctuation of crystallites were also evaluated. Result indicated that stretched molecular chains acted as nuclei while surrounding chains could contribute to the

growing crystallites. Deformation of crystal lattice with applied stress was detected and the strain-induced crystallites were found to be responsible for the increased modulus upon elongation. The unit cell volume decreased almost linearly with applied stress.

Therefore, the compressive stress in the direction perpendicular to the macroscopic stretching direction must be dominant during the deformation of strain-induced crystallites. The reinforcement effect of the crystallites is thought to be brought out not directly from crystallites connected in series but indirectly through the surrounding network chains compressing the crystallites.

### 24 - 26 September and other 5 presentations.

Effect of network-chain length on strain-induced crystallization of NR and IR vulcanizates, Kohjiya S, Tosaka M, Murakami S, Poompradub S, Ikeda Y, Toki S, Sics I, Hsiao B, The 164th Fall Technical Meeting of Rubber Division, ACS, Cleveland, Ohio, USA, 14 - 17 October.

Role of fatty acids in strain-induced crystallization of natural rubber, Tosaka M, Kyoto University Alliance for Chemistry 21st Century COE Program, Elucidation of nano structures and properties of elastomeric materials, Uji, Kyoto, 14 November.

Natural Rubber: A strategic materials and its future, Kohjiya S, 8th Pacific Polymer Conference, Bangkok, Thailand, 24 - 27 November.

Direct observation of fine structures in crystalline solids of polymers, Tsuji M, 13-th Symposium on Polymeric Materials, Kyoto, 5 December.

# **Grants**

Kohjiya S, Role of polymers in all solid-state ionic devices, Grant-in-Aid for Scientific Research, Priority Area (B), 1 April 1999 - 31 March 2004.

Kohjiya S, Stress-induced crystallization behavior of natural rubber, Grant-in-Aid for Scientific Research, (B) (3), 1 April 2003 - 31 March 2005.

Tsuji M, Analysis of internal fine structure of the high-speed spun fibers for PET/PEN blends. Grant-in -Aid fir Scientific Research (C) (2), 1 April 2002 - 31 March 2004.

# **Interface Science**- Solutions and Interfaces -

# http://kaimen.kuicr.kyoto-u.ac.jp



Prof NAKAHARA, Masaru (D Sc)



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### Visitor

Prof BARTHEL, Josef

University of Regensburg, Germany, 16 October 2003

# **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 under extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Static and dynamic NMR of endocrine disruptors, anesthetics, peptides, and proteins in lipid bilayer membranes are also investigated.

# Research Activities (Year 2003)

# **Presentations**

# Water and Solutions under Extreme Conditions

Noncatalytic Cannizzaro-type Reaction of Acetaldehyde in Supercritical Water, Nagai Y, Wakai C, Matubayasi N, and Nakahara M, International Conference on High Pressure Science and Technology, France, 7-11 July.

A Theoretical Approach to the Solvation Free Energy in the Method of Energy Representation, Matubayasi N, Molecular Liquids: Routes from Local Order to Large-Scale Cooperativity EuroConference, 5 - 10 September.

Multinuclear Magnetic Resonance Spectroscopic Study on Self-diffusion of NaCl and CsCl in Supercritical Water, Nakahara M, International Bunsen Discussion on Dynamics of Molecular Phenomena in Supercritical Fluids, Germany, 1 - 5 September, and 22 related presentations in other meetings and symposia.

### Ultra-thin Films

Structure Control of Monolayer Films by Strong Correlations between Single Amide Group and Surface Pressure, Hasegawa T [Nihon University] and Umemura J, Symposium of Grant-in-Aid for Scientific Research for Priority Areas "Dynamic Control of Strongly Correlated Soft Materials", 29 July, and 1 related presentation in other meeting.

# NMR of Membrane-Peptide Interactions

High-Resolution NMR Studies on Interactions between Peptides and Phospholipid Bilayers, Kimura T, Okamura E, Matubayasi N, and Nakahara M, Electrochemical Society

# Noncatalytic Disproportionation Reaction of Acetaldehyde in Supercritical Water

In supercritical water at 400 °C and 0.5 g/cm³ (37 MPa), acetaldehyde is found to be transformed without catalysts into ethanol and acetic acid through a disproportionation reaction. The disproportionation competes against the thermal decomposition into methane. Ethanol is generated in excess to acetic acid, and carbon dioxide appears as a product only in the presence of supercritical water. This reaction behavior is explained by considering that carbon monoxide is provided by the acetaldehyde decomposition and leads to the formation of formic acid as a reducing intermediate for acetaldehyde. [Fig. 1]

# Binding of a Neuropeptide Achatin-I to Phospholipid Bilayer

Molecular mechanism of the binding of a neuropeptide achatin-I (Gly-D-Phe-Ala-Asp) to large unilamellar vesicles of phosphatidylcholine (PC) is investigated by means of natural-abundance <sup>13</sup>C and high-resolution (of 0.01 Hz order) <sup>1</sup>H NMR spectroscopy. The binding equilibrium depends sensitively on the ionization state of the N-terminal NH3<sup>+</sup> group in achatin-I. The location of the peptide is the polar region of the PC bilayer interface. [Fig. 2] The sidechain conformational equilibria of the aromatic D-Phe and ionic Asp residues are both affected by the binding; the induced changes are attributed to the peptide-lipid hydrophobic interactions.

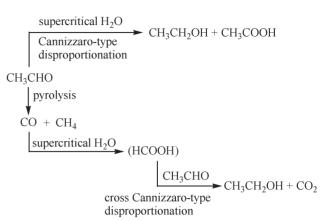
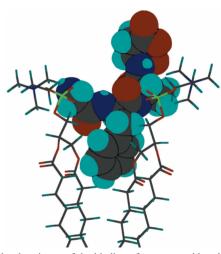


Fig. 1



**Fig. 2** Molecular picture of the binding of a neuropeptide achatin-I to phospholipid bilayer interface.

Symposium on the Chemistry of Gas-Liquid, Liquid-Liquid, and Liquid-Solid Interfaces, 18 - 19 September, and 5 related presentations in other meetings and symposia.

# **Grants**

Nakahara M, Collaboratory on Electron Correlations - Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2001 - 31 March 2006.

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 Creative Scientific Research (A) (2), 1 April 2003 - 31 March 2006.

Nakahara M, "Free-Energy Analysis of Nanoscale Ag-

gregates of Molecules in the Method of Energy Representation", National Research Grid Initiative Project, 1 April 2003 - 31 March 2008.

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

Okamura E, Transport of Endocrine Disruptors in Phospholipid Bilayer Membranes, Grant-in-Aid for Scientific Research (C) (2), 1 April 2002 - 31 March 2004.

Wakai C, Inversion of Magnitude Relation of Translational and Rotational Diffusion Coefficients for Organic Acids and Their Ions in Aqueous Solutions, Grant-in-Aid for Scientific Research for Young Scientists (B), 1 April 2002 - 31 March 2004.

# Interface Science - Molecular Aggregates -

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



Prof SATO, Naoki (D Sc)



Assoc Prof ASAMI, Koji (D Sc)



Instr KITA, Yasuo (D Sc)



Instr YOSHIDA, Hiroyuki (D Sc)

# Lecturer (pt)

Prof HIRATSUKA, Hiroshi (D Sc)

Gunma University

### **Students**

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### **Visitor**

Prof FELDMAN, Yuri Hebrew University of Jerusalem, Israel, 10 November 2003

# Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and the 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 2003)

# **Presentations**

Electron Correlation in Molecular Films: Impact on Electronic Structure of Unoccupied States, Sato N, International WE-Heraeus Seminar (No. 306) on Energetics of Interfaces between Organic Molecules and Conductors (Bad Honnef, Germany), 20 - 22 March.

Macroscopic Current-voltage Relations of Alamethicin Ion Channels, Asami K, 25th Annual Meeting of Membrane Society of Japan (Tokyo, Japan), 8 - 9 May.

Correlation Between Polymorphism and Electronic Properties of Lithium Phthalocyanine Studied on the Basis of Electronic Structures Observed for the Unoccupied States, Sato N, Tsutsumi K, Yoshida H, Sumimoto M (Dept. Mol. Eng.), Fujimoto H (Kumamoto U.), Sakaki S (Dept. Mol. Eng.), The European Conference on Organic Electronics & Related Phenomena 2003 (Wye, U.K.), 21 - 26 September.

Dielectric Spectroscopy of Colloid and Biological cells, Asami K, 2003 Autumn Meeting of Physical Society of Japan (Okayama, Japan), 20 - 23 September.

Polymorphism and Electronic Structures of Unoccupied States in Lithium Phthalocyanine Thin Films Studied using Inverse Photoemission Spectroscopy, Sato N, Tsutsumi K, Yoshida H, Fujimoto H (Kumamoto U.), Sumimoto M (Dept. Mol. Eng.), Sakaki S (Dept. Mol. Eng.), 2nd Japan-Sweden Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (Hayama, Japan), 21 - 25 October.

# **Grants**

Asami K, Manipulation of Single Biological Cells by AC Fields and Their Dielectric Spectroscopy, Grant-in-Aid for Scientific Research (C)(2), 1 April 2002 - 31 March 2004.

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.

# Direct observation of electronic structures of unoccupied states in lithium phthalocyanine thin films in relation to their polymorphism

Lithium phthalocyanine (LiPc) is a neutral radical which is stable even in the air; it has an unpaired electron deriving a singly occupied molecular orbital (SOMO) according to its Pc macrocyclic ring, and then its physical properties, in particular, its intrinsic semiconductivity and magnetic behaviors, have attracted interests of many people in the research field of organic materials science. Besides, LiPc shows polymorphism as most Pc's do and the three different polymorphs, i.e. the x-, the  $\alpha$ - and the  $\beta$ forms, of crystals have been characterized so far by several research groups. Brinkmann et al. have reported that the x-form tetragonal crystal shows a notably low electric resistivity along the molecular stacking axis and that the monoclinic α-form one exhibits a Curie-Weiss susceptibility with a mean-field temperature characteristic of ferromagnetic couplings.

In this study, LiPc thin films in the x- and the  $\alpha$ -forms were successfully prepared on gold substrates in the first place. Then their inverse photoemission (IPE) spectra were measured to examine any differences in the electronic structures of unoccupied states between two forms of the films, as the electronic structures of their valence states have been observed to be almost the same from a preliminary measurements of their ultraviolet photoemission spectra by Fujimoto *et al.* The obtained IPE spectra were interpreted with the aid of the results calculated for a LiPc molecule and its dimers in the forms corresponding to the x- and the  $\alpha$ -forms using the density functional theory (DFT) method in collaboration with Sakaki *et al.* 

The obtained IPE spectra for two kinds of the films were different from each other as shown in Fig. 1: the lowest energy feature originated from SOMO is located lower in energy for the  $\alpha$ -form film, and the second lowest energy feature corresponding to the next lowest unoccupied molecular orbital (NLUMO) appears to be much broader for the x-form one. With referring to the obtained results from the calculations above, we have come to a conclusion on the spectral interpretation as follows: the broad feature for 6e<sub>g</sub> orbital (NLUMO) for the x-form is understood by the removal of its degeneracy due to a large intermolecular interaction along the molecular stacking axis in the film, and the lower energy of  $2a_{lu}$  orbital (SOMO) for the  $\alpha$ form is explained by higher contribution of electron correlation, both Coulomb and exchange repulsions, working in the x-form film in particular. On the basis of these conclusions, the different characteristics in the electrical and magnetic properties revealed between the x- and the αforms of LiPc as mentioned above appear to be essentially elucidated to a large extent.

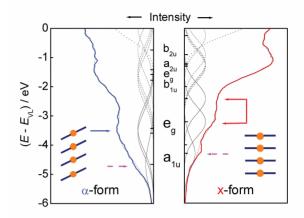


Fig. 1 Comparison of IPE spectra between the  $\alpha$ -form and the x-form of LiPc films with respective molecular stacking manners shown schematically. The ordinate is the state energy with reference to the vacuum level and as for the abscissae spectral intensities increase toward both sides. The spectral deconvolution using Gaussian functions is shown for each datum with the assignments; the arrows point the energy positions of the notable spectral features. Inserted pictures exhibit molecular stacking manners schematically.

# N-terminal insertion of alamethicin helices in voltage-activated ion-channel formation

Alamethicin, a 20-residue peptide, is supposed to form ion channels of a helix-bundle type by inserting the N-terminus into lipid bilayer membranes under sufficient voltages. In this study, the N-terminal insertion has been examined with an alamethicin dimer (di-alm) that is N-terminally linked by a disulfide bond. When di-alm was added to the cis-side membrane, it forms long lasting channels with the lifetime  $\tau$  of about 100 ms at *cis*-positive voltages. The lifetime was reduced to a few milliseconds by addition of dithiothreitol (DTT) to the cis-side membrane, indicating that most of the channels were formed by the monomers (alm-SH) resulted from the cleavage of the disulfide bond in di-alm by DTT. The succeeding addition of tetrathionate (TT) to the trans-side produced channels of  $\tau = 10-20$  ms besides the channels of alm-SH. The results suggested that TT reacted with the N-terminal thiol group of alm-SH locating at the trans-side of the membrane to alter the lifetime. The N-terminal insertion of alamethicin helices by voltage activation, therefore, was confirmed.

# Interface Science - Hydrospheric Environment Analysis -

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



Prof SOHRIN, Yoshiki (D Sc)



Assoc Prof UMETANI, Shigeo (D Sc)



Instr SASAKI, Yoshihiro (D Sc)



Instr OKAMURA, Kei (D Sc)



Assoc Instr NORISUYE, Kazuhiro (D Sc)



Techn MINAMI, Tomoharu



KINUGASA, Masatoshi (D2) EZOE, Masako (M2) NAKATSUKA, Seiji (M1)

# Visitor

Instr PENG, Xiuhong

Chengdu University of Technology, Sichuan, China, 27 October 2003 - 15 January 2004

# Scope of Research

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

# Research Activities (Year 2003)

# **Presentations**

Analysis and dynamics of trace metals in the ocean. Sohrin Y, 23rd Professor Masayoshi Ishibashi Memorial Lecture, 28 April.

Chemical oceanography by using in-situ chemical analyzers. Okamura K, The 64th conference on the Japan Society for Analytical Chemistry, 24 May 2003.

Design of solvent extraction system as separation and concentration methods for metal ions. Umetani S, The 64th conference on the Japan Society for Analytical Chemistry, 24 May 2003.

Dynamics of dissolved and dissolvable trace metals during the subarctic pacific iron experiment for ecosystem dynamics study (SEEDS 2001), Kinugasa M, Sohrin Y, Ishita T, Takeda S, Nishioka J, Tsuda A, IUGG2003, 4 July.

Zr, Nb, Hf, Ta, and W in the northwest Pacific Ocean, Sohrin Y, Mikata M, Minami T, Norisuye K, Goldschmidt Conference 2003, 12 September.

## **Grants**

Sohrin Y, Dynamics of trace bioelements in the ocean and its effect on ecosystem, Grant-in-Aid for Scientific Research (B) (1), 1 April 2001 - 31 March 2004.

Okamura K, Development of in situ measurement system of CO<sub>2</sub> related matter in seawater for global warming control, NEDO Grant, 1 April 2001 - 31 March 2004.

Okamura K, Development of time-series measurement system of sulfur related matter in seawater, Grant-in-Aid for Young Scientists B, 1 April 2003 - 31 March 2006.

### **Award**

Sohrin Y, 18th Oceanochemistry Award (Research Institute of Oceanochemistry)

# Dynamics of trace metals during the subarctic Pacific iron experiment for ecosystem dynamics study (SEEDS2001)

During the first iron-enrichment experiment in the northwest subarctic Pacific (SEEDS2001), the dynamics of dissolved and acid-dissolvable trace metals were studied. Before the Fe enrichment, the dissolved Fe concentration in the surface mixed layer was <0.13 nM (the detection limit) and the acid-dissolvable Fe concentration was 4.7 nM. The difference derived from a particulate fraction including Fe in organisms. Since the photochemical quantum efficiency of algal photosystem II was low, Fe in this fraction was not easily available to phytoplankton. After the Fe enrichment, acid-dissolvable Fe in the patch decreased from 9.6 nM on day 2 to 4.6 nM on day 13, which was still ~3 nM higher than that at the Out-patch station. Dissolved Fe was 1.4 nM on day 2 and decreased exponentially to <0.13 nM on day 11. The concentration ratio of the acid-dissolvable fraction to the dissolved fraction was lower for the other trace metals than that for Fe. The acid-dissolvable concentrations for Mn, Co, Ni, Cu, Zn and Cd did not show significant change during the observation. The dissolved concentations for Co, Ni, Cu, Zn and Cd in the surface layer on day 2 were 0.039, 5.0, 1.7, 2.2 and 0.27 nM, respectively. They decreased exponentially to 0.013, 4.3, 1.2, 0.87 and 0.21 nM on day13, respectively. The mole ratio of the concentration difference between days 2 and 13 was  $Si(OH)_4$ :  $NO_3$ :  $PO_4$ : Fe : Zn : Ni : Cu : Cd =  $27:16:1:1\times10^{-3}:1\times10^{-3}:6\times10^{-4}:4\times10^{-4}:5\times10^{-5}$ which was similar to the elemental ratio reported for phytoplankton. These are the first data showing that mesoscale iron fertilization alters the dynamics of dissolved Co, Ni, Cu and Zn.

# Distributions of dissolved and acid dissolvable bioactive trace metals in the North Pacific Ocean

Dissolved and acid dissolvable Fe, Co, Ni, Cu, Zn, Cd and Pb were measured in the North Pacific Ocean (40-17°N, 151°E-160°W) in June-July 2000.

Profiles of dissolved and acid dissolvable Fe show a large intra-basin variation. The concentrations are 0.3-1.4 nM for dissolved Fe (D Fe) and 0.7-4.7 nM for acid dissolvable Fe (AD Fe) in deep water. The concentrations are high at stations in the northwestern area and southwest off the Hawaiian Islands. AD Fe increases below 4000 m suggesting resuspension of sedimentary material. For Co, Ni, Cu, Zn, and Cd, the concentrations of dissolved and acid dissolvable species mostly agree within an experimental error. Deep water distributions of Ni, Cu, Zn, and Cd are fairly uniform in the basin. AD Pb is significantly higher than D Pb especially in surface water.

Comparison to our previous data (Fujishima et al., 2001) in the subarctic North Pacific in July-September 1997 indicates the heterogeneous distributions of the bioactive trace metals in the surface mixed layer in the North Pacific. In the subtropical region, chlorophyll biomass is very low owing to depletion of major nutrients, resulting in surface maxima of D Fe and D Zn. In the subarctic region, D Fe and D Zn are depleted in the surface mixed layer. In contrast, D Co and D Ni are high in the northwestern subarctic area and low in the subtropical gyre.

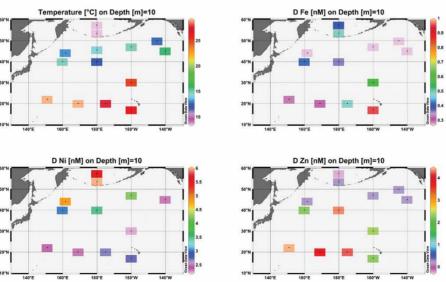


Figure. The horizontal distributions of water temperature, D Ni, D Fe, and D Zn at a depth of 10 m.

# **Solid State Chemistry** - Artificial Lattice Alloys -

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



Assoc Prof ONO, Teruo (D Sc) [Adjunct Assoc Prof]



Techn KUSUDA, Toshiyuki

### **Students**

MIYAKE, Kousaku (D3) OKUNO, Takuya (D3) OHKOCHI, Takuo (D1) JIKO, Norihiro (D1) MATSUMURA, Shigeru (M2)

# Scope of Research

Metallic thin films, multilayers, and nanostructures are prepared by ultrahigh-vacuum deposition and electron-beam lithography. Magnetic and electric transport properties are studied using various experimental techniques including Mössbauer spectroscopy, x-ray magnetic scattering, and neutron diffraction. Novel magnetic and transport properties are explored by engineering the size and shape of magnetic materials.

# Research Activities (Year 2003)

### **Presentations**

Measurement of Propagation Velocity of a Magnetic Domain Wall in a Submicron Magnetic Wire, Himeno A, Ono T, Nasu S, Okuno T, Mibu K, Shinjo T, 18th International Colloquium on Magnetic Films and Surfaces, Madrid, 22 - 25 July.

Resistance Control by Spin Current in Manganites, Kogusu A, Ono T, Nasu S, Masuno A, Terashima T, Takano M, 18th International Colloquium on Magnetic Films and Surfaces, Madrid, 22 - 25 July.

MFM Observation of Current-Driven Domain Wall Displacement in Submicron Magnetic Wires, Yamaguchi A, Ono T, Nasu S, Miyake K, Mibu K, Shinjo T, 18th International Colloquium on Magnetic Films and Surfaces, Madrid, 22 - 25 July.

Confinement of Magnetic Domain Walls at Nanocontacts between NiFe Wires or Dots, Miyake K, Shigeto K, Ono T, Shinjo T, Mibu K, 18th International Colloquium on Magnetic Films and Surfaces, Madrid, 22 - 25 July.

Magnetic Properties of Magnetic Vortex Cores in Track Shaped Magnetic Dots, Okuno T, Shigeto K, Mibu K, Ono T, Shinjo T, 18th International Colloquium on Magnetic Films and Surfaces, Madrid, 22 - 25 July.

Spin Accumulation in Ferromagnet/Superconductor/ Ferromagnet Double Tunnel Junctions, Fukuda T, Ono T, Nasu S, Okuno T, Shigeto K, Mibu K, Shinjo T, International Conference on Magnetism, Rome, 27 July - 1 August.

Weak Localization in Lacally Modulated Magnetic Field, Fuse D, Ono T, Segi T, Nasu S, Kohno H, Tatara G, Okuno T, International Conference on Magnetism, Rome, 27 July - 1 August.

Simultaneous Measurements of Magnetoresistance and Magnetic Domain Structures of L-Shaped Magnetic Wires, Yamaguchi A, Ono T, Nasu S, Miyake K, Mibu K, Shinjo T, International Conference on Magnetism, Rome, 27 July - 1 August.

Growth-Orientation Dependence of Magnetic Properties of Cr-Based Multilayers with Sn Nonatomic Layers, Jiko N, Almokhtar M, Takeda M, Suzuki J, Shinjo T, Mibu K, International Conference on Magnetism, Rome, 27 July - 1 August.

Magnetic Domain Walls and Shape-Induced Exchange Biasing Effect in NiFe Nanocontact-Structures, Miyake K, Mibu K, Ono T, Shinjo T, International Workshop on Microspectroscopy of Quantum, Magnetic and Biological Nanostructures, Osaka, 22 - 23 October.

Real-Space Observation of Current-Driven Domain Wall Displacement in Submicron Magnetic Wires, Ono T, Yamaguchi A, Nasu S, Miyake K, Mibu K, Shinjo T, International Workshop on Nano-Scale Magnetoelectronics, Nagoya, 25 - 27 November.

### **Grants**

Ono T, Dynamics of a Single Domain Wall in Artificially Structured Magnetic Wires, Grant-in-Aid for Scientific Research (C) (2), 1 April 2003 - 31 March 2005.

Ono T, Nanospintronics Design and Realizzation, MEXT Special Coodination Funds for Promoting Science and Technology, 1 September 2002 - 31 August 2005.

# **Current-Driven Domain Wall Motion due to Spin-Transfer in Magnetic Nanowires**

In conventional magnetic devices, the magnetic configuration has been controlled by a magnetic field. Here we show that spin-polarized currents can change the magnetic state through the direct interaction between electrons and magnetic moments.

In general, ferromagnets are composed of magnetic domains, within each of which magnetic moments align. The directions of magnetization of neighboring domains are not parallel. As a result, there is a magnetic domain wall (DW) between neighboring domains. The direction of moments gradually changes in a DW as shematically illustrated in Fig. 1(a). What will happen if an electric current flows through the DW? The spin direction of a conduction electron follows the local magnetic moment when the electron crosses the DW. Thus, there is a change in angular momentum of the electron (Fig. 1(b)). To conserve the total angular momentum of the system, the angular momentum sholud be absorbed by the magnetic moments in the DW. This spin-transfer creates the torque on the DW. In consequence, the electric current moves the DW.

Magnetic wires of 10 nm-thick  $Ni_{81}Fe_{19}$  were fabricated onto thermally oxidized Si substrates by means of an e-beam lithography and a lift-off method. The width of the wire is 240 nm.

Figure 2(a) shows the magnetic force microscopy (MFM) image after an introduction of a DW into the wire. The DW is imaged as a bright contrast, which corresponds to the stray field from positive magnetic charge. In this case, a head-to-head DW is realized as schematically illustrated in Fig. 1(a). After the observation of Fig. 2(a), a pulsed-current was applied through the wire in the absence of a magnetic field. The current density and the pulse duration were  $1.2 \times 10^{12}$  A/m<sup>2</sup> and 5 µs, respectively. Figure 2(b) shows the MFM image after an application of the pulsed-current from left to right. The DW moved from right to left by the application of the pulsed-current. The direction of the DW motion was reversed by switching the current polarity as shown in Fig. 2(c). The tail-to-tail DW also moved opposite to the current direction, which confirmed that the DW motion was not caused by a magnetic field generated by the current.

We can control the DW position in the wire by tuning the intensity, the duration and the polarity of the pulsedcurrent. Thus, spintronic devices, whose operation is based on the DW motion, can be directly operated by the current.

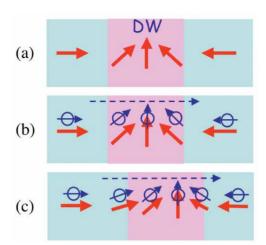


Fig. 1 Illustration of the current-driven domain wall motion due to spintransfer effect.

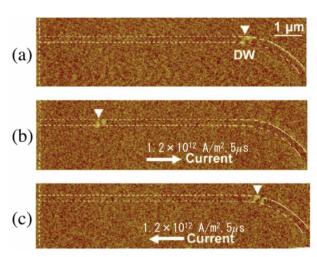


Fig. 2 Real-space observation of the current-driven domain wall motion by magnetic force microscopy.

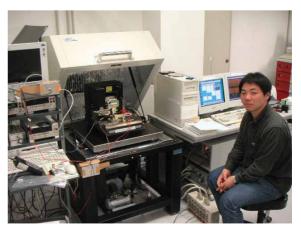


Fig. 3 Yamaguchi, A. working on MFM system.

# **Solid State Chemistry**- Advanced Inorganic Synthesis -

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



Prof SHIMAKAWA, Yuichi (D Sc)



Instr IKEDA, Yasunori

# **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 2003)

## **Presentations**

Magnetic properties of La,Co substituted *M*-type Srferrite synthesized by the polymerized complex method, Kikuchi M, Nakamura T, Nakamura M, Miki M, Nakanishi M, Fujii T, Takada J, Ikeda Y, The 91st Annual Meeting of the Society of Powder and Powder Metallurgy, Tokyo, 22 May.

Low-temperature synthesis of *M*-type hexagonal ferrite by the polymerized complex method, Kikuchi M, Nakamura T, Nakamura M, Miki M, Nakanishi M, Fujii T, Takada J, Ikeda Y, The 91st Annual Meeting of the Society of Powder and Powder Metallurgy, Tokyo, 22 May.

Magnetic properties of La,Co substituted *M*-type Srferrite synthesized by the Citrate-method, Kikuchi M, Tanaka K, Nakamura T, Nakamura M, Miki M, Nakanishi M, Fujii T, Takada J, Ikeda Y, The 92nd Annual Meeting of the Society of Powder and Powder Metallurgy, Osaka, 6 November.

Magnetic properties of Co,Sn substituted *M*-type Baferrite synthesized by the Citrate-method, Kikuchi M, Ashioka J, Nakamura T, Nakamura M, Miki M, Nakanishi M, Fujii T, Takada J, Ikeda Y, The 92nd Annual Meeting of the Society of Powder and Powder Metallurgy, Osaka, 6 November.

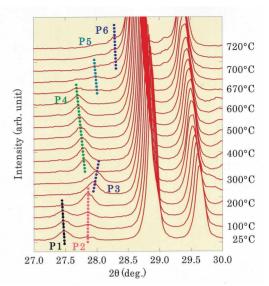
# Phase diagrammatic studies on high-*Tc* superconducting oxides

One of the most novel classes of transition-metal oxides is the high-Tc superconductors. Bi<sub>2</sub>Sr<sub>2</sub>CuO<sub>6+δ</sub> has been expected to provide crucial information about the superconducting mechanism due to its simple crystal structure and chemical composition. However, our careful phase diagrammatic studies on this compound revealed that there are at least six phases with different oxygen contents. The oxygen contents are controlled by changing the annealing temperature. The variation in oxygen contents causes changes in carrier concentration of the materials, and thus leads to the variation in superconducting transition temperature, ranging from 0 (an insulator) to 26 K.

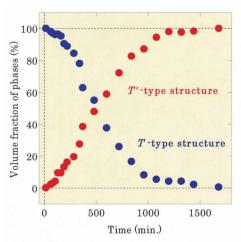
Pr<sub>2-x</sub>La<sub>x</sub>CuO<sub>4</sub> is a related compound to high-*Tc* superconducting oxides. When samples with 1.35<*x*<1.5 are quenched after annealing at 1000°C, they show a *T*-type crystal structure, which is the same as that of hole-doped La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub>. Interestingly, Pr<sub>2-x</sub>La<sub>x</sub>CuO<sub>4</sub> gradually changes its structure from *T*-type to *T'*-type, which is the typical structure for electron-doped Pr<sub>2-x</sub>Ce<sub>x</sub>CuO<sub>4</sub>, even at room temperature. Since ion diffusion in solids is extremely low at room temperature, the observed behavior is quite peculiar. It might be related to microscopic electronic phase separation, which is one of the recent key issues concerning strongly correlated electron systems.

# Novel functional oxides

In transition metal oxides, the cation-d-orbital and anion-p-orbital are strongly hybridized. Competitive and/or cooperative energies of Coulomb interaction, bandwidth, and exchange interaction also play an important role in giving rise to a wide variety of physical and chemical properties. Such exotic properties could be useful for the functions of electronic devices. There are many examples of such functional oxides: Li-ion batteries are Li-containing Co- or Ni-oxides, and FeRAMs (ferroelectric random access memories) used in IC cards consist of Pb(Zr,Ti)O<sub>3</sub> or Bi-containing Ta oxides. Recent significant developments in x-ray and neutron diffraction techniques enable us to determine the detailed crystal structures of such oxides. The information about the structures provides a basis for electronic structure calculations. Therefore, we discuss the relationships between the fundamental physics and useful functions of the functional oxides.



High-temperature x-ray diffraction patterns of  $\mathrm{Bi_2Sr_2CuO_{6+\delta}}$ . The oxygen content decreases with increasing temperature. P1 — P6 denote super-structure diffraction peaks of phases with different oxygen contents.



Phase transformation of Pr<sub>2-x</sub>La<sub>x</sub>CuO<sub>4</sub> from a *T*-type to *T*'-type structure.

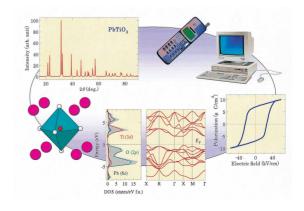


Illustration of our research processes.

# **Solid State Chemistry**- Amorphous Materials -

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



Prof YOKO, Toshinobu (D Eng)



Assoc Prof TAKAHASHI, Masahide (D Sc)



Instr TOKUDA, Yomei (D Eng)



Assoc Instr ENKHTUVSHIN, Dorjpalam



A Res MENAA, Bouzid (D Eng)



PD YAO, Jianxi (D Eng)



PD KAKIUCHIDA, Hiroshi (D Eng)



Guest Res Assoc KE, Shao (D Sc)

### **Students**

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# Scope of Research

In this laboratory, amorphous and polycrystalline inorganic materials with various optical functions such as photo-refractive, optical nonlinearity and photo-catalysis are the target materials, which are synthesized by sol-gel, multi-cathode sputtering, melt-quenching and sintering methods. In order to obtain highly functional materials the structures are investigated by X-ray diffraction techniques, high-resoluction NMR, thermal analysis, various laser spectroscopies and ab initio molecular orbital calculations.

# **Research Activities (Year 2003)**

### **Presentations**

Photochemical Process of Divalent Germanium Responsible for Photorefractive Index Change in GeO<sub>2</sub>-SiO<sub>2</sub> Glasses, Takahashi M, Sakoh A, Nishii J and Yoko T, X International Conference on the Physics of Non-Crystalline Solids, Italy, 13 - 17 July.

Organic-Inorganic Hybrid Low-Melting Glasses Consisting of Siloxane Bonds, Masai H, Takahashi M, Tokuda Y, Shimada R and Yoko T, X International Conference on the Physics of Non-Crystalline Solids, Italy, 13-17 July.

Local Structure of Lead Silicate Glasses, Mizuno M, Takahashi M, Takaishi T, Tokuda Y, and Yoko T, The 5th International Meeting of Pacific Rim Ceramic Societies Incorporating the 16th Fall Meeting of the Ceramic Society of Japan, 29 September - 2 October.

Photochemical Reactions Responsible for Photorefractive Index Change in Germanosilicate Glasses, Takahashi M, Sakoh A, Yoko T *et al*, Glass & Optical Materials Division Meeting, USA, 12 - 15 October.

Thermal and Viscoelastic Properties of Organically Modified Hybrid Low-Melting Glasses Consisting of Siloxane Framework Prepared by Sol-Gel Melting Method, Yoko T, Masai H, Menaa B *et al*, Glass & Optical Materials Division Meeting, USA, 12 - 15 October.

# Photochemical reactions responsible for photorefractive index change in GeO<sub>2</sub>-SiO<sub>2</sub> glasses

The ultraviolet-induced photochemical reactions in GeO<sub>2</sub>-SiO<sub>2</sub> glasses is widely used to manufacture fiber Bragg gratings. The photochemical reaction of the divalent Ge (Ge<sup>2+</sup>) which, we believe, is mainly responsible for the photorefractivity has been investigated by the photoluminescence spectroscopy. The excitation-emission mapping of the spectra reveals that the highly photo-active

Ge<sup>2+</sup> (PADGe) shows a large Stokes shift. This indicates that the local structure around the PADGe is allowed to relax due to the free space, resulting in the refractive index change. We have also fabricated the thermal-switching waveguide in the GeO<sub>2</sub>-SiO<sub>2</sub> thin films.

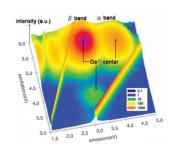
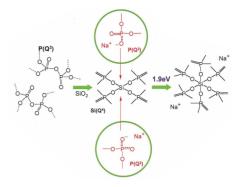


Fig. 1 A bird's-eye view of the PL spectrum mapping of as-deposited GeO<sub>2</sub>-SiO<sub>2</sub> CVD film. The intensity axis is shown in logarithm scale.

# 6-coordinated Si in phosphate glasses

It has been demonstrated that Si in some sodium phosphate glasses takes a 6-coordinated structure, while it does exist as a 4-coordinated structure in conventional oxide glasses. We have investigated the detailed local structure of 6-coordinated Si, Si(6), in the glasses and then proposed the formation mechanism by means of <sup>29</sup>Si and <sup>31</sup>P MAS NMR spectroscopy and ab initio molecular orbital (MO) calculations. The ratios of an increment of P with 3 bridging-oxygens, P(Q3), to that of Si(6) were determined as about 2, indicating that the formation of one Si(6) needs two P(3)'s. The ab initio MO calculations have shown that the energy of a model with Si(6) octahedrally coordinated by six P(Q3)'s is lower than that of Si tetrahedrally coordinated

dinated by four P(3)'s, Si(4) by 1.9eV. Therefore, Si(6) is more stable in sodium phosphate glasses than Si(4).

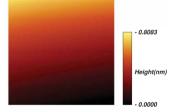


**Fig. 2** Formation mechanism of a local structure of 6-coordinated Si, Si(6). The stabilization energy of a cluster with Si(6) has been calculated as 1.9eV.

# Preparation of organic/inorganic low-melting glass thick-films

Pollutant-free low-melting glasses are considered to have potential applications in the active optical devices. Recently, we have developed organic/inorganic hybrid low-melting glasses by the sol-gel melting method. Thick

films of over 10  $\mu$ m can be obtained using dipcoating method. The absolute roughness of the film has been determined as  $8.5*10^{-4} \mu$ m by AFM. The propagation loss of film has been also measured as less than 1 dB/cm at 1553 nm.



**Fig. 3** Atomic force microscopy topography for low-melting glass. The observed area is  $50 * 50 \mu m$ . The film thickness is  $3.25 \mu m$  and the absolute roughness is  $8.5*10^4 \mu m$ 

# **Grants**

Yoko T, Photochemical reactivity of glasses, Grantin-Aid for Scientific Research (A) (2), 1 April 2001 - 31 March 2005.

Takahashi M, Development of photorefractive low-melting glasses, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2005.

Takahashi M, Development of photonics materials based on the organic-inorganic hybrid low melting glasses, PRESTO, Japan Science and Technology, 1 November 2002 - 31 October 2005.

# Award

TAKAHASHI M, Japan-Australasian Ceramic Society Joint Ceramic Award, Study on the Optical Functional Glasses Doped with Active Centers, The Ceramic Society of Japan and Australasian Ceramic Society, 30 May 2003.

# Fundamental Material Properties - Molecular Rheology -

# http://molrheo.kuicr.kyoto-u.ac.jp



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Visitor

Prof VLASSOPOULOS, Dimitris

FORTH and University of Crete, Greek, 20-25 March 2003

# Scope of Research

The molecular origin of various rheological properties of materials is studied. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluids 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 autocorrelation of the orientation with dynamic dielectric spectroscopy.

# Research Activities (Year 2003)

### **Presentations**

Tensile Properties of Transparent PC-PDMS Elastomers, Inoue T, ISE2003, 3 April.

Electric Birefringence and Viscoelasticity of Amorphous Polymers, Inoue T, Annual Meeting of the Society of Polymer Science Japan, 15 May.

Electric Birefringence and Viscoelasticity of Amorphous Polymers, Kadoya H, Annual Meeting of the Society of Rheology Japan, 15 May.

Rhology of Carbon Black Systems, Aoki Y, Discussion Meeting of the Society of Rheology Japan, 16 September.

Viscoelasticity of Living Polymers, Oishi Y, Discussion Meeting of the Society of Rheology Japan, 16 September.

Birefringence and Viscoelasticity of Branching Polymers, Matsuno K, Discussion Meeting of the Society of Rheology Japan, 17 September.

Relationship Between Viscoelastic Relaxation Function and Intermediate Scattering Function for Entangled Linear Chain in Early Stages of Tube Dilation Process, Paul A KR, Discussion Meeting of the Society of Rheology Japan, 17 September.

Equilibration of Bridge Population in Block Copolymer Mixed Lamella Systems, Tan H, Discussion Meeting of the Society of Rheology Japan, 17 September.

Rheo-dielectric behavior of poly(ethylene oxide) containing lithium perchlorate, Matsumiya Y, Annual Meeting of the Society of Rheology, 13 October.

Dielectric and viscoelastic behavior of polyisoprene blends: Test of tube dilation mechanism, Watanabe H, Annual Meeting of the Society of Rheology, 14 October.

Electric Birefringence of Amorphous Polymers, Inoue T, Slow Dynamics in Complex Systems, 8 November.

### Grant

Paul A KR, Development of a Model for Entanglement Dynamics of Polymers Having Multiple Coarse-graining Scales, Grant-in-Aid for Scientific Research, 1 April 2003 - 31 March 2004.

### Award

Kadoya H, Award for the Best Presentation, Electric Birefringence of Amorphous Polymers, The Society of Rheology Japan, 15 May.

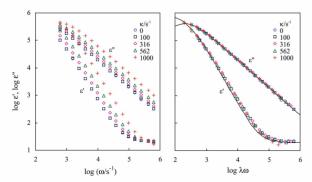
# Rheo-dielectric Behavior of Poly(ethylene oxide) Melts Containing Lithium Perchlorate

Electrical properties of polymer electrolyte systems have been extensively investigated. However, many problems remain for the properties under flow. For a model electrolyte, polyethylene oxide (PEO; M = 1000) melt containing lithium perchlorate (LiClO<sub>4</sub>) at the Li:ethyleneoxide molar ratio of 1:10), we have examined the dielectric behavior at equilibrium as well as under steady shear flow [1].

At the shear rate  $\kappa=0$  (at equilibrium), the PEO/LiClO<sub>4</sub> system exhibits significant dielectric dispersion attributable to the electrode polarization of Li<sup>+</sup> ions; see left panel of Figure where the dielectric constant  $\epsilon$ ' and dielectric loss  $\epsilon$ ' are plotted against angular frequency  $\omega$ . These Li<sup>+</sup> ions form intermolecular bridging of the PEO chains to constrain the chain motion, as evidenced from a significant increase in the zero-shear viscosity  $\eta_0$  upon addition of LiClO<sub>4</sub> to PEO.

Under shear, the  $\epsilon$ ' and  $\epsilon$ " curves shift to higher  $\omega$  with increasing  $\kappa$ , and a master curve is obtained when the frequency is normalized with a shift factor  $\lambda$  (< 1); see right panel. These rheo-dielectric features indicate that the flow enhances the ionic mobility  $\mu$  by the factor of  $1/\lambda$  but induces no change in the ion concentration. Indeed, the rheo-dielectric data are well described by the Macdonald theory for the electrode polarization [2] combined with the flow-induced increase of  $\mu$ ; see solid curves in right panel of Figure. Furthermore, the PEO/LiClO<sub>4</sub> system exhibited strong shear thinning of the viscosity  $\eta$  with increasing  $\kappa$  and the magnitude of thinning ( $\eta/\eta_0$  ratio) coincided with the dielectric shift factor  $\lambda$ . This coincidence reflects a strong motional cooperativity between the PEO chain segment and Li<sup>+</sup> ion.

- Y. Matsumiya, N. P. Balsara, J. B. Kerr, T. Inoue, and H. Watanabe, Macromolecules, 37, 544 (2004).
- 2. J. R. Macdonald, Phys. Rev., 92, 4 (1953).



Rheo-dielectric behavior of  $PEO/LiClO_4$  system at  $25^{\circ}C$ . Solid curves in the right panel indicate the prediction of the Macdonald theory.

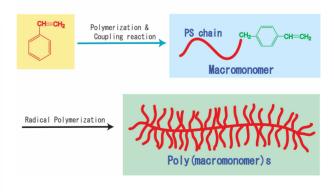
# **Rheo-Optics of Poly(macromonomer)s**

Molecular theories for polymer chain dynamics are based on the concept of statistical segments. For the case of polystyrene, the estimated molecular weight of the segment is approximately 1000, which means one segment conposed of about ten repeating units. Recently, physical properties of new types of polymers having highly branching architecture, like dendrimers and poly(macromonomer)s, have attracted a lot of attention. For such polymers, it is not clear how the concept of the segment should be modified because the distance of the branching points is shorter than the segment size for linear polymers.

When a amorphous polymers is deformed, it becomes anisotropic and birefringent. The strain-induced birefringence reflects the internal stain, and therefore simultaneous measurement of the stress and the birefringence, rheo-optical method, is a useful technique to understand molecular origin of the stress and its relaxation mechanism. [1,2]

Recently, we have synthesized a series of polystyrene poly(macromonomer) and have measured the birefringence and simultaneously the Young's modulus. Comparing with the ordinary linear polystyrenes, we have found that the stress-optical coefficient for poly(macromononer) significantly reduced with increasing of molecular weight of macromonomers (500<M<3000). This result can be attributed to the reduction of the segment size. Thus, we may conclude that the segment size, defined as a unit supporting the entropic stress, is significantly reduced for poly(macromonomer)s. This effect has not been realized untill this study and cannot be well understood from our present knowledge for linear polymers.

- 1. T. Inoue, H. Okamoto and K. Osaki, Macromolecules, 24, 5670(1991).
- 2. T. Inoue and K. Osaki, *Macromolecules*, **29**, 1595(1996).



 $Synthesize \ of \ styrene \ poly(macromonomer)s.$ 

# **Fundamental Material Properties**- Polymer Materials Science -

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



Prof KANAYA, Toshiji (D Eng)



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# 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 intention 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 2003)

### **Presentations**

Electrolyte and Non-electrolyte Behavioral Boundary in Polyelectrolyte Solutions, Nishida K, Kaji K, Kanaya T, The 2nd NIST-KIPS Symposium on Polymer Science, Gaithersburg, USA, 21 March.

Structure and Dynamics of Polymer Networks As Revealed by Scattering Techniques, Takahashi N, Kanaya T, Nishida K, Kaji K, 9th International Seminar on Elastomers, Kyoto, 2 April.

Inelastic Neutron Scattering Studied on Ultra Thin Polymer Film, Inoue R, Yamano H, Nishida K, Kanaya T, Tsukushi I, Shibata K, Autumn Meeting, The Physical Society of Japan, Okayama, 22 September.

Mesomorphic Phase Formation and Crsytallization of Polypropylene, Konishi T, Nishida K, Kanaya T, Kaji K, Autumn Meeting, Society of Polymer Science, Japan, Yamaguchi, 24 September.

Crystallization of Isotactic Polypropylene under Shear Flow - Effect of Shear Rate and Strain -, Ogino Y, Takahashi N, Matsuba G, Sharma L, Nishida K, Kanaya T, Kaji K, Autumn Meeting, Society of Polymer Science, Japan, Yamaguchi, 24 September.

The Effect of Phase Separation on Crystal Nucleation for Polyolefin Blends, Matuba G, Shimizu K, Wang H,

Wang Z, Han C C, Autumn Meeting, Society of Polymer Science, Japan, Yamaguchi, 25 September.

Polymer Crystallization Under Shear Flow, Kanaya T, European Discussion Meeting on Polymer Physics, Waldau, Germany, 26 September.

# **Grants**

Nishida K, Control of higher order structures of polymer materials by a rapid temperature jump method, Industrial Technology Research Grant Program by New Energy and Industrial Technology Development Organization (NEDO) of Japan, 1 April 2001 - 31 March 2004.

Kanaya T, Sharma L, Production of an artificial bone material based on a hydroxyapatite polymer base, involving polyurethane hybrids, Grant-in-Aid for Scientific Research (JSPS Fellows), 15 April 2002 - 15 April 2004.

Kanaya T, Nishida K, Polymer Crystallization under Shear Flow - Aiming to Reveal the Formation Mechanism of Fiber Structure, Grant-in-Aid for Scientific Research (B) (2), 1 April 2003 - 31 March 2005.

Kanaya T, Tasaki S, Dynamics of Graft Polymer Chains in Nanometer Scale by Neutron Spin Echo, Grant-in-Aid for Exploratory Research, 1 April 2003 - 31 March 2005.

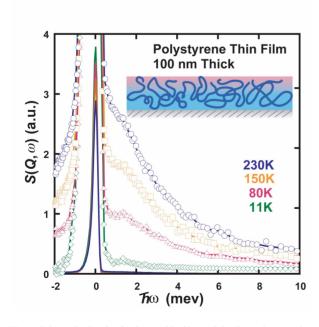
# **Inelastic Neutron Scattering on Polymer Thin Films**

Properties of polymer thin films and/or polymer surfaces are very different from those of the bulk and related to many phenomena such as adhesion, wetting, surface friction, and hence are important from viewpoints of not only science but also industrial applications. Aiming to elucidate the special nature of thin films and/or surfaces, we have investigated the thermal expansion behavior of polystyrene (PS) thin films using X-ray reflectivity (XR) as well as dynamics of PS thin films using an inelastic neutron scattering technique. One of the most interesting findings in this study is reduction of thermal expansivity in the glassy state with deceasing the film thickness. Onset thickness of the reduction is very close to twice of the radius of gyration of a polymer chain, suggesting that it is originated from the confinement effects of a polymer chain. In order to elucidate the origin of the reduction of the expansivity, we performed inelastic neutron scattering measurements on PS thin films 100 and 40 nm thick below the glass transition temperature  $T_{g}$  (=373 K). The observed dynamic scattering laws  $S(Q,\omega)$  are shown in Figure 1. Analyzing the spectra, we found that the mean square displacement  $\langle u^2 \rangle$  decreases with the film thickness, suggesting the reduction of the expasivity is caused by stressinduced hardening of polymer chains.

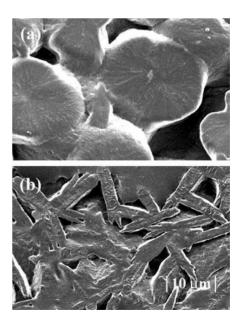
# Novel Crystal Morphology Generated by Crystallization from Meta-stable State

When polymers in bulk are crystallized quiescently by thermal processing, crystal aggregates of spherical silhouette are usually formed, which are well known as "spherulite". So it is rare case that polymer crystal has special morphology other than spherulite. Although, isotactic polypropylene (iPP) has been known as a typical polymer forming spherulite (Figure 2(a)), we have succeeded in generating novel iPP crystals having "bamboo leaf-like (BL) morphology (Figure 2(b)) by a rapid temperature jump technique.

When the molten iPP is rapidly quenched with a rate faster than 80 °C / sec, it solidifies in a meta-stable state, the so-called mesomorphic phase. It is said that the structure of the mesomorphic phase is liquid crystal like, but the details of it are still in discussion. When the mesomorphic iPP was heated up to a certain temperature near melting temperature, the BL crystals were found. The BL crystals grew until the good part of matrix was run out and micro~meso voids were left. The BL crystals showed higher crystallinity than the ordinary spherulites. Thus, the polymer crystallization passing through a meta-stable state has a potential to control higher order structure of polymer materials.



**Fig. 1** Schematic sketch of polymer thin film and the dynamic scattering law  $S(Q,\omega)$  of polystyrene thin film 100 nm thick.



**Fig. 2** Scanning electron microscope (SEM) images of iPP crystals. (a): ordinary spherulites. (b): typical BL crystals.

# **Fundamental Material Properties**- Molecular Dynamic Characteristics -

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



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# Associate Instructors (pt) Dr TSUNASHIMA, Yoshisuke

Dr ISHIDA, Hiroyuki

### **Visitors**

Dr AMORNSAKCHAI, Taweechai Prof HU, Shaohua Prof LAUPRETRE, Francoise Mr CHAIYUT, Nattawut Mahidol University, Tailand, 17 March - 11 April, 2003 Donghua University, China, 22 April - 25 April, 2003 CERMAV, France, 4 May - 17 May, 2003 Mahidol University, Tailand, 19 May - 18 August, 2003

# Scope of Research

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

# Research Activities (Year 2003)

# **Presentations**

Nanoassembly Structure and Its Changes of Bacterial Cellulose, Horii F, 225th ACS National Meeting, 24 March (Invited).

Multidimensional Multiple-Quantum NMR Analyses of Local Structures in Solid Polymers, Kaji H, 52th Annual Meeting, Soc. Polym. Sci., Jpn., 28 May (Invited).

AFM Observation of Band-like Cellulose Assemblies Produced by *Acetobacter Xylimum*, Hirai A, Tsujii Y, Tsuji M, Horii F, 52th Annual Meeting, Soc. Polym. Sci., Jpn., 28 May.

Structure of Nano-Assemblies of Bacterial Cellulose Produced in the Presence of Fluorescent Brightener with Different Concentrations, Tsujitani K, Hirai A, Horii F, Tsuji M, Annual Meeting, Cellulose Soc. Jpn, 18 July.

Solid Structure and Dynamics of Polymers - Recent Research Progress, Horii F, 52th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 24 September (Invited). Structure of Band-like Cellulose Assemblies Produced by *Acetobacter Xylinum*, Hirai A, Horii F,Tsujii Y, Tsuji M, 52th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 24 September.

Structure Analyses of Polymer Organic EL Materials by Solid-State NMR Spectroscopy, Kaji H, Onoyama G, Tsukamoto N, Horii F, 52th Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 25 September.

Structures and Dynamics of Carrier Transport Materials in Organic EL Devices, Kaji H, Tsukamoto N, Yamada T, Horii F, 42th NMR Conf. Jpn., 26 November.

### **Grants**

Kaji H, Higher Order Structures and Optical Properties of Light-Emitting Polymeric Materials, PRESTO, Japan Science and Technology Agency, 1 November 2002 - 31 October 2005.

Hirai A, Preparation and Structural Analysis of Bacterial Cellulose/Natural Inorganic Nanocomposites, Grant-in Aid for Scientific Research (C)(2), 1 April 2003 - 31 March 2005.

# Sine-Modulated Two-Dimensional Pure Exchange Solid-State NMR as a Tool for Characterizing Dynamics in Solids

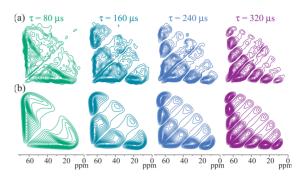
We present a simple two-dimensional (2D) solid-state exchange NMR method to suppress significant undesirable diagonal signals, termed 2D sine-modulated pure exchange (2D SIMPREX). Two delays, τ, incorporated in standard 2D exchange experiments modulate the 2D spectra with  $\sin\{(\Omega_1 - \Omega_2)t\}$ , where  $\Omega_1$  and  $\Omega_2$  are precession frequencies corresponding to y- and x-axes of 2D spectra, respectively. A demonstration for dimethyl sulfone (DMS), (CH<sub>3</sub>)<sub>2</sub>SO<sub>2</sub>, is shown in Fig. 1. The diagonal signals are successfully suppressed by incorporating the sine-modulation, which results in clear detection of 108° reorientation motion of CH<sub>3</sub> groups in DMS. Another demonstration is given for polyethylene, by combining this technique with magic angle spinning. Not only the exchange signals between the crystalline and noncrystalline components but also those among the noncrystalline components in different states, which could not be detected so far, are clearly observed. The 2D SIM-

# AFM Observation of Cellulose Assemblies Produced by *Acetobacter Xylinum*

TEM, AFM and X-ray diffraction studies revealed the crystal structure and higher order structures of cellulose assemblies produced by *Acetobacter xylium* under different culture conditions. TEM, however, gave only two-dimensional structural information of the specimen. Recently, we have succeeded in obtaining three-dimensional structural information by combining AFM and TEM observations. Fig. 2a shows a TEM photograph of band-like cellulose assembly on the TEM grid. Fig.2b shows an AFM image of the same band-like cellulose assembly on the same grid. The height of band-like cellulose assemblies was estimated to be 20-30 nm from their AFM height profiles as shown in Fig. 2c. The crystallite sizes in the band-like cellulose

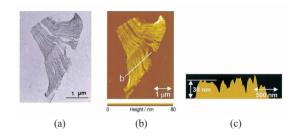
# **Inorganic-Organic Molecular Hybrid Materials** with Polyoxometalate Cores

Antimonate, a kind of polyoxometalate, is expected to use as core or building block for inorganic-organic nanohybrid materials because surface oxygens have high basicity.  $[Sb_4O_6(OH)_4\{OSi(CH_3)_2(t-C_4H_9)\}_6]^{2-}$  anion (1) was successfully prepared by the reaction of octaantimonate  $[Sb_8O_{12}(OH)_{20}]^4$  with t-butyl dimethyl silanol and the detailed structure was clarified by solid-state NMR. In contrast, other silanols seem not to react with octaantimonate in a similar way and the specific antimonate frame may be destroyed. Substitution reactions were, therefore, examined between the silanol residues and other silanols for anion 1. As a result, two vinyl silanols  $C_2H_3Si(CH_3)_2OH$  were found to be introduced at the top and bottom sites as shown in Fig. 3, which was obtained by single-crystal X-ray diffractome-



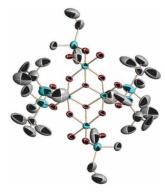
**Fig. 1** (a) Experimental 2D SIMPREX spectra of DMS at 23 °C. (b) Simulated spectra for (a) with reorientation angle of 108°. Both the positive and negative signals are shown as solid lines. The mixing time is 50 ms.

PREX techniques enable us to efficiently identify and analyze the dynamics in solid materials, which are difficult to be detected so far due to the overlap with huge diagonal artifacts.



**Fig. 2** (a) TEM photo of band-like cellulose assembly. (b) AFM image of band-like cellulose assembly on the TEM grid. (c) Height profile along the line b in Fig. 2b.

assembly were estimated from the X-ray diffraction analysis. A structural model of the band-like cellulose assembly was proposed on the basis of these results.



**Fig. 3** Structure of  $[Sb_4O_6(OH)_4\{OSi(CH_3)_2(C_2H_3)\}_2\{OSi(CH_3)_2(t-C_4H_9)\}_4]^{2-}$  anion (2).

try. Further reactions associated with the vinyl groups of anion (2) are in progress.

# **Organic Materials Chemistry**- Polymeric Materials -

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



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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 high-density polymer brushes (HDPB).

# **Research Activities (Year 2003)**

### **Presentations**

2 presentations, The 1st Trilateral Warkshop on Organic Chemistry, Taiwan, 17 - 19 Jan.

Structure and Properties of HDPB (Invited Lecture), Fukuda T, and 2 other presentations, The 2nd NIST-KIPS Symposium on Polymer Science, USA, 20 - 21 Mar.

Structure and Properties of HDPB (Invited Lecture), Tsujii Y, and 3 other presentations, 225th ACS National Meeting, USA, 23 - 27 Mar.

Formation of Branched Polymer Systems by LRP (Invited Lecture), Fukuda T, and 1 other presentation, 9th International Seminar on Elastomers, Kyoto, 2 - 4 Apr.

Synthesis and Properties of Newly Developed Polymer Brushes (SPSJ Willey Award Lecture), Tsujii Y, Soc. Polym. Sci., Jpn., 25 Sep.

8 presentations, Spring Meeting, Soc. Polym. Sci., Jpn., 28 - 30 May.

3 presentations, Polymer Symposium, Soc. Polym. Sci., Jpn., 10 Jul.

8 presentations, Autumn Meeting, Soc. Polym. Sci., Jpn., 24 - 26 Sep.

3 presentations, Annual Meeting, Soc. Fib. Sci. Tech., Jpn., 11 - 13 Jun.

### **Grants**

Fukuda T, Science and Technology of HDPB, Grantin-Aid for Science Research (A)(2), 1 Apr 2002 - 31 Mar 2005.

Tsujii Y, Fundamental Study on HDPB, Grant-in-Aid for Science Research (B)(2), 1 Apr 2002 - 31 Mar 2005.

Tsujii Y, Nanostructre Control by Mixed Polymer Brushes, Grant-in-Aid for Exploratory Research, 1 Apr 2003 - 31 Mar 2005.

Ohno K, Gold Nanoparticles Coated with HDPB, Grant-in-Aid for Young Scientists (B), 1 Apr 2002 - 31 Mar 2004.

Goto A, Chain Length Dependence of  $k_t$ , Grant-in-Aid for Yound Scientists (B), 1 Apr 2003 - 31 Mar 2005.

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

Kaya K, Collaboratory on Electron Correlations, Grantin-Aid for Cre. Sci. Res., 1 Apr 2001 - 31 Mar 2006.

### **Award**

Tsujii Y, SPSJ Willey Award for 2003, Synthesis and Properties of Newly Developed Polymer Brushes, Soc. Polym. Sci, Jpn., 25 Sep 2003.

### Fabrication of Ordered Arrays of Gold Nanoparticles Coated with High-Density Polymer Brushes

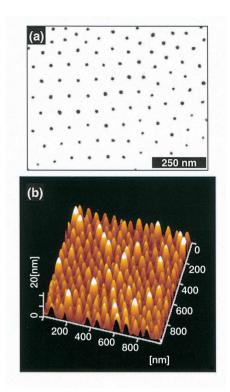
By means of surface-initiated LRP, we have synthesized a metal-polymer hybrid which has the core of the gold nanoparticle (AuNP) prepared by a simple one-pot method with a narrow size distribution, and the shell of the poly(methyl methacrylate) (PMMA) end-grafted on the core surface with a surface density as high as about 0.4 chains/nm<sup>2</sup> and a controlled chain length and chain length distribution. Primarily due to the high surface density, the PMMA grafts at the air-water interface exert interparticle interactions of an extremely long range, a range comparable to the full length of the PMMA chain. As a result, we have succeeded for the first time in fabricating a two-dimensional array of the AuNPs with a high degree of structural order and an exceptionally wide controllability of the interparticle distance (Figure 1). Owing to the simplicity and versatility of surface-initiated LRP, this work may be extended to other metal and semiconductor nanoparticles for their 2D and 3D ordered assemblies with wide controllability of lattice parameters.

K. Ohno, K. Koh, Y. Tsujii, T. Fukuda, Angew. Chem. Int. Ed., **42**, 2751-2754 (2003). This paper was awarded the status of a Hot Paper by Angewandte Chemie.

# Precision Synthesis of Organic/Inorganic Hybrid Nanocapsule with Silanol-Functionalized Micelle Template

A novel technique is presented for the construction of a silica-based capsule of tens of nanometers size (Figure 2). An amphiphilic block copolymer carrying several protected silanol groups near the free end of the hydrophilic block was synthesized by the copper-mediated LRP (ATRP) in conjunction with the sequential monomer addition technique. In an aqueous media, the amphiphile formed a micelle with a diameter about 40 nm with the silanol groups populated near the micelle surface. Mixing the micelle with an active silicate solution at ph 9 formed a silica layer with a thickness of several nanometers on the micelle surface, thus producing a new type of organic/inorganic hybrid nanocapsule composed of the core of a polymeric micelle and the shell of a silica thin layer (Figure 3).

K. Koh, K. Ohno, Y. Tsujii, T. Fukuda, Angew. Chem. Int. Ed., **42**, 4194-4197 (2003). This paper was awarded the status of a Very Important Paper by Angewandte Chemie.



**Figure 1.** (a) TEM and (b) AFM micrographs of the transferred films of AuNP-PMMA hybrid:  $M_0$  of the PMMA graft = 28 000.

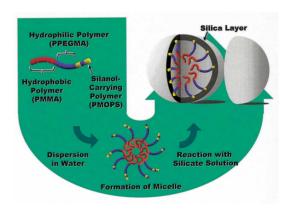


Figure 2. Strategy for the synthesis of an organic/inorganic hybrid nanocapsule.

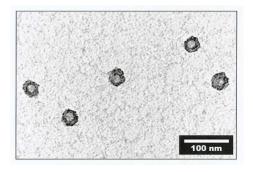


Figure 3. TEM image of the organic/inorganic hybrid nanocapsule.

## **Organic Materials Chemistry** - Organic Structural Chemistry -

### http://133.3.40.20/



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### Scope of Research

Fundamental studies are being conducted for creation of new functional materials with novel structures and properties. The major subjects are: synthetic and structural studies on novel cyclic  $\pi$ -conjugated systems, particularly the positively charged species stabilized by  $\sigma$ - $\pi$  interaction; synthesis of new redox-active and supramolecular  $\pi$ -systems; organochemical transformation of fullerene  $C_{60}$ , specifically the synthesis of fullerene dimers and trimers by the use of mechanochemical solid-state reactions; synthesis and reactions of open-cage fullerene derivatives; generation of alkylated C<sub>60</sub> cation and its application for synthesis of functional materials.

### Research Activities (Year 2003)

### **Presentations**

Synthesis of Open-Cage Fullerene Derivatives and Encapsulation of Small Molecules, Komatsu K, Murata Y, Murata M, The 203rd Meeting of the Electrochemical Society, 28 April, Paris, France.

Generation and Properties of Functionalized Fullerenyl Cations, Kitagawa T, Lee Y, Murata Y, Cheng F, Komatsu K, 225th ACS National Meeting, 24 March, New Orleans, USA.

Radical Cations and Dications of Oligothiophene Annelated with Rigid σ-Frameworks, Nishinaga T, Komatsu K et al., Gordon Research Conferences on Physical Organic Chemistry, 29 June, Laconia, USA.

Synthesis and Electrolytic Polymerization of a Fullerene-Terthiophene Dyad, Murata Y, Suzuki M, Yamazaki T, Komatsu K, The 203rd Meeting of the Electrochemical Society, 2 May, Paris, France.

### Grants

Komatsu K, Appearance of biradical character in  $\pi$ -conjugated hydrocarbons by annelation with strained bicyclic frameworks, Grant-in-Aid for Scientific Research (B) (2), Apr. 2002 - Mar. 2004.

Kitagawa T, Grant-in-Aid for Scientific Research (C) (2), Apr. 2002 - Mar. 2004.

Nishinaga T, Grant-in-Aid for Young Scientists (B), Apr. 2002 - Mar. 2004.

Murata Y, Grant-in-Aid for Young Scientists (B), Apr. 2002 - Mar. 2004.

Kitagawa T, CREST, Japan Science and Technology Corporation, Nov. 2002 - Oct. 2007.

Murata Y, Komatsu K, Academic-Industrial Cooperative Research Fund, Aug. 2002 - Mar. 2004.

### Stable Radical Cations and Dications of Oligothiophenes Surrounded by Bicyclo[2.2.2]octene Units

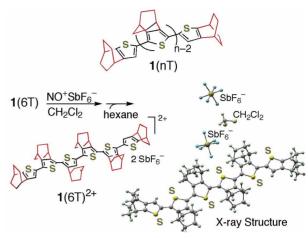
Oligothiophenes 1 annelated with bicyclo[2.2.2]octene (abbreviated as BCO) units were designed and synthesized in order to elucidate the uni-molecular properties of cationic oligothiophenes.[1] The radical cation salts of the dimer and trimer and dication salts of the tetramer and hexamer have been isolated as air-stable single crystals and their structures have been determined by X-ray crystallography. In these crystals, the effective inhibition of intermolecular  $\pi$ - $\pi$  interaction by BCO units was shown,[2] indicating that 1 is a suitable system for the investigation of the properties of longer oligomer dications, the unimolecular magnetic properties of which (singlet, triplet, or independent biradicals) are still controversial.

### Electron-Transfer Induced Substitution of Alkylated $C_{60}$ Chlorides with Proton Sponge

A series of alkylated  $C_{60}$  chlorides 2 were found to undergo rapid substitution with proton sponge 3, affording donor-acceptor dyads 4 in good yields.[3] A chain mechanism, initiated by a single-electron transfer from 3 to 2, is proposed on the basis of the results of rate measurements. This is the first example of the  $S_{RN}1$  reaction observed for alkylated  $C_{60}$  chlorides. The facility of such a reaction is reasonably anticipated from the inherent electronegativity of the fullerene core, which was demonstrated by the reduction potential and low LUMO energy of 2. The present result provides a novel practical method to synthesize fullerene—donor dyads using a variety of electron-rich aromatic compounds.

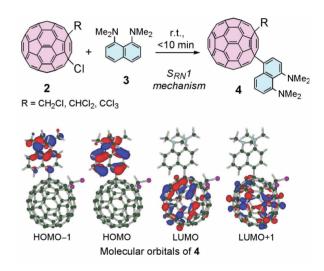
## 100% Encapsulation of Molecular Hydrogen in an Open-Cage Fullerene

We succeeded in the synthesis of a fullerene derivative 5 having a 13-membered ring orifice in 40% overall yield based on consumed  $C_{60}$  by three-step organic reactions, i.e., a reaction of  $C_{60}$  with a 1,2,4-triazine derivative, photochemical oxidation, and insertion of a sulfur atom on the rim of the orifice.[4] A 100% encapsulation of molecular hydrogen in 5 was achieved for the first time by treating solid 5 at 200 °C under 800 atmosphere of hydrogen for 8 hours. Furthermore, when the hydrogen containing molecule,  $H_2@5$ , was subjected to MALDI-TOF MS at a high laser power,  $H_2@5$  transformed its structure to  $H_2@C_{60}$  by itself in the gas phase. This could be taken as the first step

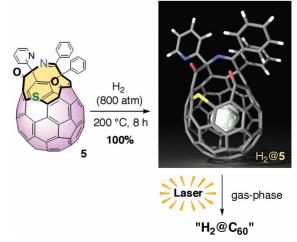


1. Wakamiya A, Yamazaki D, Nishinaga T, Kitagawa T, Komatsu K, J. Org. Chem., 2003, 68, 8305.

2. Nishinaga T, Wakamiya A, Yamazaki D, Komatsu K, J. Am. Chem. Soc., 2004, 126, in press.



3. Kitagawa T, Lee Y, Komatsu K, J. Org. Chem., 2004, 69, 263.



4. Murata Y, Murata M, Komatsu K, Chem. Eur. J., 2003, 9, 1600.

5. Murata Y, Murata M, Komatsu K, J. Am. Chem. Soc., 2003, 125, 7152.

# Synthetic Organic Chemistry - Fine Organic Synthesis -

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



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### Scope of Research

The research interests of the laboratory include the development of new synthetic methodology, 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 selective reactions, synthesis of unusual amino acids, visualization of molecular chirality by functionalized phenolphthalein, use of homooxacalixarene for molecular recognition, and the structural and functional investigation of heterochiral oligomers.

### Research Activities (Year 2003)

### **Presentations**

A Facile Asymmetric Synthesis of Tetrahydro-isoquinoline and Tryptoline Derivatives with a Quaternary Carbon Center at C(3), Ozturk O, Shimada S, Kawabata T, Fifth AFMC International Medicinal Chemistry Symposium, 14 October.

Memory of Chirality in Intramolecular Alkylation of Amino Acid Derivatives: A Facile Synthesis of Chiral Nitrogen-Containing Heterocycles, Kawabata T, Kawakami S, Majumdar S, Ozturk O, 15th International Symposium on Chirality, 22 October.

Effective Synthesis of Optically Active Naphthalene Oligomers, Tsubaki T, Miura M, Morikawa H, Tanaka H, Furuta T, Tanaka K, Kawabata T, Fuji K, 15th International Symposium on Chirality, 22 October.

New C<sub>2</sub>-Symmetric PPY Analogues as Catalysts for Enantioselective Acylation, Schedel H, Kawabata T, The Nineth International Kyoto Conference on New Aspects of Organic Chemistry, 10 November.

Asymmetric Induction Based on Dynamic Chirality

of Enolates, Kawabata, T, The 2nd Takeda Science Foundation Symposium on PharmaSciences, 2 December.

### **Grants**

Kawabata T, Design of a New Generation of Nucleophilic Catalysts and Selective Reactions, Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2005.

Tsubaki K, Visualization of Molecular Information using Phenolphthalein Derivatives. Grant-in Aid for Scientific research (C) (2), 1 April 2002 - 31 March 2004.

Kawabata T, Majundar S, Asymmetric Cyclization based on the Dynamic Chirality of Enolates, Grant-in-Aid for Scientific Research, 31 October 2003 - 30 October 2005.

Kawabata T, Schedel H, Development of a New Generation of Chiral Nucleophilic Catalysts, Grant-in-Aid for Scientific Research, 3 June 2003 - 2 June 2005.

### **Award**

MIURA M, Best Poster Award, Effective Synthesis of

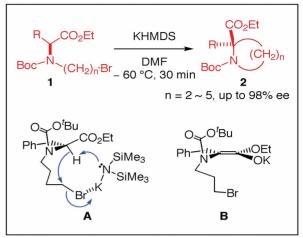
## **New Protocol for Asymmetric Cyclization of Amino Acid Derivatives**

N-( $\omega$ -Bromoalkyl)- $\alpha$ -amino acid derivatives 1, readily prepared from natural  $\alpha$ -amino acids, gave cyclic amino acids with a quaternary stereocenter by treatment with KHMDS in DMF. Chirality of the parent amino acids was almost completely preserved during an enolate-formation and cyclization process, giving aza-cyclic amino acids in up to 98% ee in retention of configuration. This method is applicable to the asymmetric synthesis of azetidine (n=2), pyrrolidine, (n=3), piperidine (n=4), and azepane (n=5) derivatives. Mechanistic investigation indicated that the asymmetric cyclization proceeds via an axially chiral enolate intermediate ( $\bf B$ ), and not through a concerted  $\bf S_E$ i process ( $\bf A$ ).

## C<sub>2</sub>-Symmetric PPY Analogues as Catalysts for Enantioselective Acylation

Combinatorial synthesis of  $C_2$ -symmetric pyrrolidino-pyridine (PPY) analogues was accomplished by condensation of key intermediate  $\bf 3$ , obtained from L-glutamic acid, and variety of amino acid derivatives. A representative structure is shown as  $\bf 4$ . Catalyst  $\bf 4$  showed higher enantioselectivity than the corresponding mono-substituted PPY surrogate in asymmetric acylation of alcohols. Desymmetrization of meso-1,2-diol  $\bf 5$  with isobutyric anhydride in the presence of  $\bf 5$  mol% of  $\bf 4$  at room temperature gave  $\bf 6$  in in 75% yield and in 93% ee. Transition-state hydrogen bonding between substrate  $\bf 5$  and an acylpyridinium intermediate generated from  $\bf 4$  was suggested to be critical for the asymmetric induction.

### **Effective Synthesis of Optically Active Naphthalene Oligomers**



Kawabata T, Kawakami S, Majumdar S, *J. Am. Chem. Soc.* **2003**, *125*, 13012-13013.

Tsubaki K, Miura M, Morikawa H, Tanaka T, Kawabata T, Furuta T, Tanaka K, Fuji K, *J. Am. Chem. Soc.*, **2003**, *125*, 16200-16201.

Chiral Oligo-Naphthalene Derivatives, 9th Summer Meeting on Functional Host-Guest Chemistry (Fukuoka),

21 Aug. 2003.

## **Bioorganic Chemistry** - Organoelement Chemistry -

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



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### **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 resemblance and difference in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting 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 2003)**

### **Presentations**

Synthesis and Properties of the First Disulfur and Diselenium Complexes of Platinum, Tokitoh N, Nagata K, Takeda N, The 10th International Symposium on Inorganic Ring Systems, 17 - 23 August, Vermont, U.S.A.

Structure and Reactivity of Kinetically Stabilized Silaaromatic Compounds, Shinohara A, Takeda N, Tokitoh N, 50th Symposium on Organometallic Chemistry, 28 - 30 September, Osaka, Japan.

Recent Progress in the Chemistry of Stable Silaaromatic and Related Species, Tokitoh N, Kyushu International Symposium on Physical Organic Chemistry IX, 30 September - 3 October, Fukuoka, Japan.

### Grants

Tokitoh N, Studies on the synthesis, structures, properties, and functions of novel aromatic compounds containing heavier group 14 elements, Grant-in-Aid for Scientific Research (A)(2), 1 April 2002 - 31 March 2005.

Tokitoh N, Synthesis of dynamic complexes containing heteroatoms by taking advantage of kinetic stabilization, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2002 - 31 March 2006.

Tokitoh N, Synthesis of metallacyclopropabenzenes derivatives by using bulky substituents and the elucidation of their properties, Grant-in-Aid for Exploratory Research, 1-April 2003 - 31 March 2004.

Kawai Y, Development of methods for the determination of the absolute configuration of chiral compounds using a novel crystalline agent, Grant-in-Aid for Scientific Research (C)(2), 1 Apr 2003 - 31 March 2005.

Takeda N, Synthesis of double bond species between group 10 metals and chalcogens and the elucidation of

## Photochemical valence isomerization reaction of kinetically stabilized 9-silaanthracene

In recent decades, there has been much interests in the chemistry of  $[4n+2]\pi$ -electron ring systems containing heavier group 14 elements, *heavy aromatics*, from the viewpoint of not only fundamental chemistry but also applied chemistry. Recently, we have succeeded in the synthesis and characterization of the first stable *heavy aromatics*, that is, silabenzene, 1- and 2-silanaphthalene, 9-silaanthracene, germabenzene, and 2-germanaphthalene utilizing an efficient steric protection group, Tbt group (vide infra). In addition, we have reported the photochemical isomerization of the silabenzene leading to the corresponding silabenzvalene derivative. Now, we investigated photochemical reaction of the 9-silaanthracene 1.

When a C<sub>6</sub>D<sub>6</sub> solution of 1 in a sealed tube was irradiated with light of  $\lambda = 300-500$  nm through a UV cut filter at room temperature, the orange color of 1 dissappeared and a new species, 9,10-Dewar-9-silaanthracene 2 was formed exclusively. 2 was found to undergo gradual thermal tautomerization into 1 even at -180 °C in hexane. Kinetic studies using UV/vis spectroscopy suggested that this reaction was a first-order reaction as well as thermal isomerization of 9,10-Dewar-anthracenes to anthracenes. In addition, the half-life time of 2 in hexane at 10 °C was estimated to be about 5 minutes. On the other hand, heating of a C<sub>6</sub>D<sub>6</sub> solution of 1 at 110 °C in a sealed tube for 15 days or thermolysis of 1 in the solid state at 180 °C for 1 h afforded the corresponding [4+4]dimmer 3. 3 is thermally very stable and no cycloreversion to 1 was observed in the 1,2-dichlorobenzene- $d_4$  solution even at 200 °C.

These results are very interesting because it was experimentally demonstrated for the first time that 9-silaan-thracene can afford either the Dewar-type isomer or [4+4] dimer depending on the reaction conditions.

their properties, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.

Nagahora N, Syntheses, structure, and properties of novel low-coordinated species of heavier main group elements, Grant-in-Aid for JSPS Fellows, 1 April 2003 - March 2005.

### **Awards**

Tokitoh N, The Chemical Society of Japan Award for Creative Work, Synthesis of Aromatic Species Containing a Heavier Group 14 Element by Taking Advantage of



Right: in C<sub>6</sub>D<sub>6</sub>



# The first examples of stable benzenes fused with two three-membered rings: synthesis and structures of the two stereoisomers of bis(silacyclopropa)benzenes

Structures and properties of cyclopropabenzene derivatives have fascinated many organic chemists so far, because a competition between preservation of aromatic ring skeleton and angular strain in the three-membered ring fused to their aromatic ring results in unique properties. Recently, we have succeeded in the synthesis of the first stable diaryl sila- and germacyclopropabenzenes, heavier analogues of a cyclopropabenzene derivative, and reported their structures and physical properties. Now, we describe the synthesis of two stereoisomers of the first stable bis-(silacyclopropa)benzenes, in which two silacyclopropene skeletons are fused to one benzene ring.

The reaction of dilithiosilane **4**, which was prepared by the exhaustive reduction of dibromosilane **5** using lithium naphthalenide, with 1,2,4,5-tetrabromobenzene at -78 °C in THF afforded the first stable bis(silacyclopropa)benzenes **6a** (cis-form) and **6b** (trans-form). The structures of **6a,b** were revealed by the X-ray crystallographic analysis. It was found that both of **6a,b** have no distinct bond alternation in their central benzene rings.

Tbt Si Br 
$$(5 \text{ eq.})$$
 Tbt Li Br  $-78 \,^{\circ}\text{C}$   $6a + 6b$ 

Tbt Dip Si Si Dip Si Charlet Dip Si Dip Si Charlet Dip Si Dip Tbt: R = R' = CH(SiMe\_3)\_2

6a: cis-form, 6b: trans-form Dip Dip: R = CHIMe\_2, R' = H

Kinetic Stabilization, The Chemical Society of Japan, 20 March 2003.

Tokitoh N, Humboldt Research Award, Systematic Studies on Homo- and Heteronuclear Doubly Bonded Compounds between Heavier Group 15 Elements, Alexander von Humboldt Foundation, 7 November 2003.

Takeda N, Progress Award in Silicon Chemistry, Japan, Stabilization of Low-coordinated Group 14 Element Compounds by Taking Advantage of Steric Protection, The Society of Silicon Chemistry, Japan, 18 October 2003.

## **Bioorganic Chemistry** - Bioactive Chemistry -

http://www.scl.kyoto-u.ac.jp/~sugiura/index2.html



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### **Students**





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### **Scope of Research**

The major goal of our laboratory is to elucidate the molecular basis of the activity of various bioactive substances by biochemical, physicochemical, and synthetic approaches. These include studies on the mechanism of sequence-specific DNA cleavage by antitumor or carcinogenic molecules, studies on the DNA recognition of zinc-finger proteins, and model studies on the action of ion channels. In addition, artificial designed peptides have also been developed as useful tools in molecular biology and potentially in human medicine.

### Research Activities (Year 2003)

### **Presentations**

Artificial zinc finger proteins: Design strategy and gene action, Sugiura Y, Annual meeting, Pharm. Soc. Jpn., Nagasaki, 28 March.

Nine-zinc finger protein: influence of TFIIIA-type linker at N- or C-terminal on DNA binding site, Nomura W, Sugiura Y, 11th International Conference on Biological Inorganic Chemistry, Cairns (Australia), 23 July.

Intercellular delivery of histidine-tagged protein, Futaki S, Niwa M, Wakako N, Nakase I, Shiraishi Y, Sugiura Y, Fifth AFMC International Medicinal Chemistry Symposium, Kyoto, 14 October.

Arginine-rich peptides: The aspects of membrane translocation, Futaki S, Cellular Drug Transport Mechanisms Workshop, Molndal (Sweden), 14 November.

### **Grants**

Sugiura Y, Regulation of cellular gene function by novel DNA bending finger, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2004.

Sugiura Y, Role of multi-zinc fingers in gene expression and creation of their architectures, Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2005.

Futaki S, Development of new cellular modifier using membrane transmission peptides and analysis of proteinprotein interaction, Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2004.

### Effects of Length and Position of Extended-Linker on Sequence-Selective DNA Recognition of Zinc Finger Peptides

The new zinc finger peptides with extended-linker seuquece for recognition of noncontiguous DNA targets have been created (Figure 1). Sp1GG series are linkerextended mutants for the wild-type Sp1(zf123) and two to four amino acids are inserted into their linker sequences between finger units. From the analyses of the DNA binding affinity and specificity by gel mobility shift assay, it is clearly indicated that Sp1GG series bind to noncontiguous DNA targets with sequence-selectivity according to the position of the extended-linker (Figure 2). Moreover, the N-terminal finger substitution revealed that the linkerextended mutants bind to DNA selectively in synergy of three finger units. This is the first method for the recognition of the noncontiguous DNA target by zinc finger peptide. Consequently, our design method is widely applicable to creating zinc finger peptides with novel DNA sequenceselectivity.

W. Nomura, Y. Sugiura, Biochemistry, 42, 14805-14813 (2003).

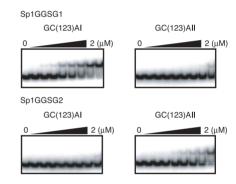
## **Basic-Peptide Mediated Protein Delivery into Living Cells**

Basic-peptide mediated protein delivery into living cells is becoming recognized as a potent approach for the understanding of cellular mechanisms and drug delivery. We have demonstrated that these features were observable among many arginine-rich peptides including octaarginine (Arg)8. The presence of a ubiquitous internalization mechanism for arginine-rich oligopeptides has also been suggested. On the other hand, there are many non-covalent protein complexes or supramolecular assemblies that have great potential for the research in chemical and cellular biology. It has never been demonstrated whether a protein assembly with a dissociation constant in the range of  $10^{-5} \sim 10^{-6}$  M is able to cross the membrane with retention of its structure.

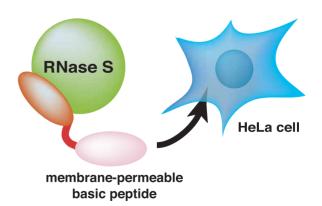
We have prepared the conjugates of the S-peptide (1 - 15) derived from RNase S with membrane-permeable basic peptides such as the human immunodeficient virus (HIV)-1 Rev (34 - 50), HIV-1 Tat (48 - 60) and octaarginine. The RNase S complexes, formed among these S-peptide (1 - 15)/basic peptide conjugates, efficiently penetrated into the HeLa cells. Moreover, these RNase S complexes

Zf123GG Series Figure 1. Finger 2 Finger 3 Finger 1 Zf123GG1 GG GGS Zf123GGS1 GGSG Zf123GGSG1 (ii) Zf123GG2 Series Finger 1 Finger 2 Finger 3 Zf123GG2 GG GGS Zf123GGS2 Zf123GGSG2 GGSG

Figure 2.



exerted an anti-HIV replication activity. The present study exemplified the applicability of the arginine-rich peptides to the intracellular targeting of non-covalent assemblies for intracellular applications.



**Figure 3.** Intracellular delivery of non-covalent protein complexes

# **Bioorganic Chemistry** - Molecular Clinical Chemistry -

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



Prof UEDA, Kunihiro (D Med Sc)



Assoc Prof TANAKA, Seigo (D Med Sc)



PD (COE) TAKEHASHI, Masanori

### **Guest Scholars**

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### **Guest Research Associate**

GRIVAS, Paul

### Lecturer (pt)

FUKUI, Kiyoshi (D Med Sc)

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### **Students**

CHEN, Liping (D4) OYANAGI, Hiroki (D4) TAKANO, Emiko (RF) TAKAGI, Jumpei (RS)

### **Visitors**

Mr ALIOTO, Tyler University of California, Berkeley, U.S.A., 2 June 2003 - 3 June 2003 Mr LIU, Timothy Stanford University, U.S.A., 7 July 2003 - 10 September 2003

### Scope of Research

This laboratory was founded in 1994 with the aim of linking (bio)chemical research and clinical medicine. Thus, the scope of our research encompasses the structure, function and pathophysiological significance of various biomolecules and bioreactions in relation to human diseases, and the application of molecular techniques to clinical diagnosis and therapy. Our current interest is focused on the role of poly(ADP-ribosyl)ation in protection of genome from apoptosis-inducing stresses, and the molecular etiology of neurodegenerative disorders including Alzheimer's disease and Parkinson's disease.

### Research Activities (Year 2003)

### **Presentations**

The Establishment of Evidence-Based Genetic Testing in Japan, Ueda K, 10th Annual Meeting of the Japanese Society for Gene Diagnosis and Therapy, Osaka, 24 - 25 July.

Role of Poly(ADP-ribose) Synthetase in Neuronal Cell Death, Tanaka S, Japanese-German Biochemistry Meeting, Marburg, 29 - 30 September.

Functional Characterization of Septin 3, Takehashi M, Japanese-German Biochemistry Meeting, Marburg, 29 - 30 September.

Poly(ADP-ribose) Synthetase Activation and Mitochondrial injury in Neuronal Cell Death, Tanaka S, and Ueda K, 76th Annual Meeting of Japanese Biochemical Society, Yokohama, 15 - 18 October.

Characterization of Novel Mammalian Septin, SEPT 3, Takehashi M, Tanaka S, Suzuki K, Nagai H, Maeda M, Kinoshita N, and Ueda K, 76th Annual Meeting of Japanese Biochemical Society, Yokohama, 15 - 18 October.

Development of Highly Sensitive *In Situ* Hybridization and RNA Amplification Methods, Iida S, Onaka S, Takehashi M, Hayashi T, TanakaS, and Ueda K, 76th Annual Meeting of Japanese Biochemical Society, Yokohama, 15 - 18 October.

### Grant

Tanaka S, Suppression of neuronal cell death by poly(ADP-ribose) synthetase inhibitors, Japan Foundation for Applied Enzymology, 1 April 2003 - 31 March 2004.

## Role of Poly(ADP-ribose) Synthetase in Neuronal Cell Death

Poly(ADP-ribose) synthetase (PARS) is a nuclear enzyme that, upon activation by DNA single-strand breaks, forms (ADP-ribose)n chains from  $\beta$ -nicotinamide adenine dinucleotide (NAD<sup>+</sup>) on acceptor proteins, including histones and PARS itself. Poly(ADP-ribose) is known to be involved in various physiological and pathological events such as DNA repair, cell differentiation, cell cycle, and cell death. The excessive activation of PARS leads to depletion of cellular NAD<sup>+</sup>. The depletion of NAD<sup>+</sup>, a co-enzyme in energy metabolism, results in reduction of ATP generation, while ATP is used for replenishment of NAD<sup>+</sup>. This "energy crisis" is considered to be causative of apoptotic and necrotic cell death.

We studied, using models derived from primary cell cultures of rat brain, role(s) of PARS in the neuronal cell death in Alzheimer's disease (AD) and cerebral infarction. In the AD model, cortical neurons became mostly apoptotic after exposure to A $\beta$  amyloid fibrils. The A $\beta$ fibrils treatment enhanced mitochondrial generation of reactive oxygen species (ROS). In the cerebral infarction model, cortical neurons became partly apoptotic and partly necrotic after oxygen-glucose deprivation. This treatment induced mitochondrial membrane depolarization and the opening of permeability transition pore (PTP), through which apoptotic factors such as cytochrome c and apoptosis-inducing factor (AIF) were released. In both AD and cerebral infarction models, PARS was activated in a dose- and time-dependent manner, resulting in the decrease of NAD<sup>+</sup> content. Addition of PARS inhibitors such as 1,5-dihydroxyisoquinoline and benzamide suppressed NAD<sup>+</sup> depletion, and also attenuated the mitochondrial injury. These in vitro models strongly suggest that PARS activation plays a critical role in the ROS-mediated neuronal cell death in the pathological conditions such as AD and cerebral infarction.

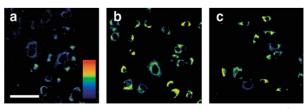
### **Functional Characterization of Septin 3**

Septin 3 is a novel member of the septin subfamily with GTPase domain. The septin 3 gene was originally cloned with a phenotype of up-regulation during neuronal differentiation of the human teratocarcinoma cell line NT2. Septin 3 has, at least, two isoforms, A and B, that are produced by the alternative splicing of a single transcript. We studied the physiological and pathological roles of septin 3 isoforms. Using antibodies specific for the isoforms A and B, we found that both isoforms were abundantly expressed in normal human brain. We further investigated intracel-

lular localization and interaction of the two isoforms in HeLa cells, transfected separately or together, by use of the antibodies in immunohistochemistry and immunoprecipitation. Both isoforms A and B were found to form fibrous structures in the cytoplasm, and the structures were to be composed of homologous as well as heterologous isoforms of septin 3. We also analyzed a genetic association of septin 3 polymorphisms with Alzheimer's disease (AD), Parkinson's disease (PD), and Lewy body variant (LBV) of AD. Genotyping of microsatellite polymorphisms in exon 11 indicated a significant difference in long/short allelic distribution between AD and control, suggesting a role played by septin 3 in pathogenesis of AD, but not PD or LBV.

## Overexpressiom of CYP2D6 Attenuates the Toxicity of MPP<sup>+</sup> in Actevity Dividing and Differentiated PC12 Cells

Clonal pheochromocytoma cell lines overexpressing cytochrome P450 2D6 (CYP2D6) were established. CYP2D6 was localized in the endoplasmic reticulum, and its enzymatic activity in the microsomal fraction was confirmed by using high performance liquid chromatography analysis with [guanidine-<sup>14</sup>C]debrisoquine as a substrate. Overexpression of CYP2D6 protected cells against the toxic effects of 1-methyl-4-phenylpyridinium ion (MPP<sup>+</sup>) at the concentration range of 20~40 µM, as assessed by the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. Further, reactive oxygen species generation was suppressed in the mitochondria. The cytotoxicity of 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) was unchanged in cells overexpressing CYP2D6 versus mock-transfected controls at concentrations up to 500 μM. These results suggest that the lowered enzyme activity of CYP2D6 in individuals, termed "poor metabolizers" may represent a risk factor from exposure to select neurotoxicants.



**Figure 1.** Mitochondrial generation of ROS after exposure to MPP<sup>+</sup>or MPTP.

Clonal cells were treated with a reduced form of chloromethyltetramethylrosamine before (a) after a 24-h incubation with 20  $\mu$ M MPP<sup>+</sup> (b) or 500  $\mu$ M MPTP (c). Mitochondrial ROS are visualized by oxidized chloromethyltetramethylrosamine (Scale bar = 40  $\mu$ m).

## **Molecular Biofunction** - Chemistry of Molecular Biocatalysts -

### http://biofun.kuicr.kyoto-u.ac.jp



Prof SAKATA, Kanzo (DAgr)



Assoc Prof HIRATAKE, Jun (D Agr)



Instr MIZUTANI, Masaharu (D Agr)



Instr SHIMIZU, Bun-ichi (D Agr)

### Lecturer (pt)

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### **Students**

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OHNISHI, Toshiyuki (D1) SAINO, Hiromichi (M2) KUBOTA, Yasuhiro (M1) KOBAYASI, Yuriko (UG)

SAITO, Shigeki (D2) KAWASHIMA, Tomoko (M2) UNO, Tetsuya (M2) YAMAGUCHI, Hikaru (M1)

### 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) Chemical, biochemical and molecular biological studies on diglycosidases specifically hydrolyzing the β-glycosidic bond between disaccharides and aglycons. 2) Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ-glutamyltranspeptidase and γ-glutamylcysteine synthetase. 3) Design and synthesis of novel inhibitors of glycosidases and their application to affinity chromatography and biological probes to understand the physiological roles of glycosidases. 4) X-ray crystallographic analysis of pyruvate phosphate dikinase from maize. 5) Directed evolutional studies of *Pseudomonas* lipase. 6) Mechanism of the activation/ inactivation process of plant hormones by cytochromes P450. 7) Molecular mechanism of regulation of phenylpropanoid pathway in plants subjected to various stresses.

### Research Activities (Year 2003)

### **Presentations**

Presentations from each project (1 - 7) are as follows:

- 1) Glycosidases in tea leaves, which may improve the flavor quality of CTC black tea, Sakata K, 3rd International Conference on Global Advances in Tea Science, Kolkata (India), 20-23 November.
- 2) y-Phosphono glutamate analogs as mechanism-based inhibitors of γ-glutamyltranspeptidase, Hiratake J, Tachi N, Suzuki H, Kumagai H, Sakata K, 9th International Kyoto Conference on New Aspects of Organic Chemistry, 13 No-
- 3) Synthesis of cyclic glycosylamidine derivaives as β-N-acetylglucosaminidase inhibitor, Uno T, Kato M, Hiratake J, Sakata K, 2003 Annual and 431st Meeting of Kansai Branch of Jpn. Soc. Biosci. Biotech., and Agrochem., 5 October.
- 4) X-Ray crystallographic study on PPDK from maize, Nakanishi T, Nakatsu T, Matsuoka M (Nagoya Univ.), Sakata K, Kato H, 2003 Annual Meeting Jpn. Soc. Biosci,

Biotech., and Agrochem., 1-3 April.

- 5) Directed evolution of lipase -Altering the reaction specificity and screening, Hiratake J, 3rd Combinatorial Bioengineering Symposium, 24 January.
- 6) Characterization of cytochromes P450 involved in ABA catabolism, Saito S, Matsumoto C, Hirai N, Ohigashi H, Ohta D, Mizutani M, Sakata K, 38th Annual Meeting Jpn. Soc. Chem. Reg. Plants, 29-30 October.
- 7) Metabolic profiling of coumarins in morning glory, *Ipomoea tricolor*, after various stresses, Kai K, Shimizu B, Sakata K, 30th Annual Meeting of Plant Growth Regulation Society of America, 3-6 August.

### **Grants**

Sakata K, Clarification of a new group of plant diglycosidase family, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Sakata K, Investigation of the floral aroma formation elicited by leaf-hopper feeding in Formosa Oolong Tea,

### ABA catabolism by P450s

Abscisic acid (ABA) is a sesquiterpene plant hormone and is involved in a number of critical processes in normal growth and development as well as in adaptive responses to environmental stresses. The hydroxylation at the 8'-position of ABA has been known as the key step of ABA catabolism, and this reaction is catalyzed by ABA 8'-hydroxylase, a cytochrome P450 (P450) (Scheme 1). We have demonstrated CYP707As as the P450s responsible for the 8'-hydroxylation of (+)-ABA. First, CYP707A cDNAs were cloned from Arabidopsis and used for the production of recombinant proteins in insect cells using a baculovirus system. The insect cells expressing CYP707A3 efficiently metabolized (+)-ABA to yield phaseic acid (PA), the isomerized form of 8'-hydroxy-ABA. The micorsomes from the insect cells exhibited very strong activity of 8'-hydroxylation of (+)-ABA ( $K_m = 1.3 \mu M$  and  $k_{cat} = 15 \min_1$ ).

## Design and synthesis of novel inhibitors of glycosidases

Glycosidases, one of the largest enzyme family, are composed of a number of enzymes with different substrate specificity and reaction mechanisms. Therefore the design of selective glycosidase inhibitors requires careful considerations for both substrate specificity and reaction mechanism of the glycosidase. We have developed β-glycosylamidines 1 as highly potent and selective inhibitors of  $\beta$ -glycosidases. The  $\beta$ -glycosylamidines, readily synthesized from sugars in two steps, serve as a highly inhibitory substrate analog ( $K_i \le 0.1 \mu M$ ) which inhibits each β-glycosidase selectively according to the glycon substrate specificity of the enzyme. This property was used successfully for the preparation of tailor-made affinity adsorbent 2 for the purification of glycosidases according to their glycon substrate specificity. We recently synthesized the cyclic glucosylamidine 3 which served as a highly potent and selective inhibitor of family 20 β-N-acetylglucosaminidases (IC<sub>50</sub> = 0.17  $\mu$ M). This

Grant-in-Aid for Scientific Research (B) (2), 1 April 2003 - 31 March 2005.

Hiratake J, Bio- and organic chemical studies on glycosidases by using transition-state and substrate analogue inhibitors as a tool, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Hiratake J, All-inclusive analysis of plant glycosidases by using specific inhibitors as a tool, Grant-in-Aid for Exploratory Research, 1 April 2003 - 31 March 2004.

Mizutani M, Analysis of the gene clusters involved in

Scheme 1. The oxidative catabolic pathway of ABA

The solubilized CYP707A3 protein bound (+)-ABA with the binding constant  $K_s = 3.5 \, \mu\text{M}$ , but did not bind (-)-ABA. Detailed analyses of the reaction products confirmed that CYP707A3 does not have the isomerization activity of 8'-hydroxy-ABA to PA. The transcripts of CYP707A genes increased in response to salt, osmotic and dehydration stresses as well as ABA. These results establish that CYP707As play a key role in regulating the ABA level through the 8'-hydroxylation of (+)-ABA.

was because the compound **3** was positively charged and structurally analogous to the oxazoline intermediate, a cyclic reaction intermediate unique to this family of glycosidases. Compound **3** did not inhibit the conventional  $\beta$ -glycosidases which are inhibited potently by the generic glycosylamidine **1**. Interestingly, the acyclic imidazolosugar **4**, which was readily formed by isomerization of **3**, served also as highly potent and selective inhibitor of family 20  $\beta$ -*N*-acetylglucosaminidases ( $K_i = 0.5 \mu M$ ). The mechanism of inhibition, the structural elaboration and applications of these glycosidase inhibitors are studied actively in this laboratory.

plant terpenoid biosynthesis, Grant-in-Aid for Young Scientist B, 1 April 2003 - 31 March 2005.

### **Awards**

Kato M, Poster Award, Glycosylamidines as Potent and Selective Glycosidase Inhibitors, 1st International Symposium on Biomolecular Chemistry (ISBC2003), 5 December.

Saito S, Poster Award, Characterization of Cytochromes P450 Involved in ABA Catabolism, 38th Annual Meeting of Jpn. Soc. Chem. Reg. Plants, 30 October.

# **Molecular Biofunction**- Molecular Microbial Science -

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



Prof ESAKI, Nobuyoshi (D Agr)



Assoc Prof YOSHIMURA, Tohru\* (D Agr)



Assoc Prof KURIHARA, Tatsuo (D Eng)

Guest Research Associate LIN, Lian-Bing



Instr MIHARA, Hisaaki (D Agr)



A Res KAZUOKA, Takayuki (D Eng)

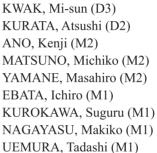
**Technicians (pt)** 



Guest Res Assoc WEI, Yun-Lin

TANAKA, Yumi HAYASHI, Misa

## Students



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MURAMATSU, Hisashi (D2)
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MATSUO, Yoko (M2)
WATANABE, Shingo (M2)
ITO, Kosuke (M1)
MURAI, Ken (M1)

OMORI, Taketo (M1) WU, Hui-Yuan (RS)

### **Visitors**

Dr PILON, Marinus Dr PILON-SMITS, Elizabeth

UTSUNOMIYA, Machiko

Colorado State University, USA, 1 November 2003 - 6 November 2003 Colorado State University, USA, 1 November 2003 - 6 November 2003

### Scope of Research

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

### Research Activities (Year 2003)

### **Presentations**

Structure and function of a novel enzyme catalyzing asymmetric reduction of a carbon-carbon double bond, Kurata A, Kurihara T, Kamachi H, Esaki N, 2003 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 1 April.

Regulation of the activity of eukaryotic serine racemase by ATP and Mg<sup>2+</sup>, Yoshimura T, Okubo F, Wu H, Esaki N. 2003 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 1 April.

Construction of protein overproduction system using a cold-adapted microorganisms as a host, Kurihara T, Wei Y, Hayashi M, Esaki N. 2003 Annual Meeting, Soc. Biotech. Jpn., 16 September.

Identification of iron-sulfur proteins by differential

screening using an IscS-deficient strain, Yamane M, Mihara H, Kurihara T, Takahashi Y, Yoshimura T, Esaki N, 2003 Annual Meeting, Jpn. Biochem. Soc., 16 October.

### **Grants**

Esaki N, Construction and functional analysis of composite biocatalysts, Grant-in-Aid for Scientific Research on Priority Areas (B), 1 April 2001 - 31 March 2004.

Esaki N, Elucidation of the mechanisms of activation of an essential trace element, selenium, and its co-translational incorporation into polypeptide chains, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2005.

Esaki N, Isolation of novel cold-adapted microorganisms and exploitation of useful gene resources, Grant-

## Protein Overproduction at Low Temperatures with a Cold-Adapted Microorganism

We have constructed a novel host-vector system for the production of proteins at low temperatures using a cold-adapted microorganism as a host. This system is particularly useful for the production of thermolabile proteins.

A cold-adapted bacterium, *Acinetobacter* sp. strain no. 6, was isolated from Siberian tundra soil. The bacterium grew well at low temperatures as low as  $4^{\circ}$ C. We have constructed an *Escherichia coli - Acinetobacter* sp. strain no. 6 shuttle vector by using a replicon from a plasmid isolated from a mesophilic *Acinetobacter calcoaceticus* strain and established an efficient transformation method by electroporation. A powerful promoter that functions in this cold-adapted bacterium was isolated by screening of the genomic DNA library with a promoter probe vector harboring a  $\beta$ -lactamase gene as a reporter. When a thermolabile  $\alpha$ -amylase gene from a cold-adapted bacterium, *She*-

## Thiolation of tRNA Catalyzed by IscS and MnmA

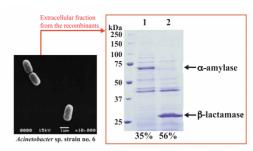
Escherichia coli tRNA contains nucleosides modified with sulfur. A sulfur-containing nucleoside, 5-methylaminomethyl-2-thiouridine (mnm<sup>5</sup>s<sup>2</sup>U), is found at the wobble position 34 of tRNA<sup>Lys</sup>, tRNA<sup>Glu</sup>, and tRNA<sup>Gln</sup>. The 2-thio group of 2-thiouridine stabilizes the anticodon structure, confers ribosome-binding ability to tRNA and improves reading frame maintenance. Recent studies showed that the biosynthesis of 2-thiouridine requires both MnmA and cysteine desulfurase IscS. However, the mechanism of the thiolation reaction has not been clarified. We cloned the mnmA gene from E. coli and overproduced and purified the gene product. The purified protein exists as monomers and dimers when determined by gel filtration chromatography. The protein catalyzed the incorporation of <sup>35</sup>S from [<sup>35</sup>S]-L-cysteine into tRNA<sup>Lys</sup> in the presence of IscS and ATP. We

in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2005.

Yoshimura T, Physiological role of D-amino acids in eukaryote, Grant-in-Aid for Scientific Research (C), 1 April 2002 - 31 March 2004.

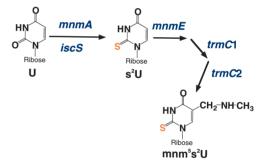
Kurihara T, Bioconversion of fluorinated organic compounds: catalytic mechanisms of elimination and incorporation of fluorine and their application, Grant-in-Aid for Young Scientists (A), 1 April 2002 - 31 March 2005.

Mihara H, Mechanisms of incorporation of sulfur and selenium into the anticodon wobble bases of tRNAs, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31



**Figure 1.** Production of extracellular  $\alpha$ -amylase (lane 1) and  $\beta$ -lactamase (lane 2) at 7°C by recombinant *Acinetobacter* sp. strain no. 6.

wanella sp. Ac10, was expressed under the control of the newly isolated promoter, the recombinant *Acinetobacter* sp. strain no. 6 secreted the  $\alpha$ -amylase, which amounted to about 35% of the total extracellular proteins. This makes a striking contrast to an *E. coli* expression system, which did not produce a detectable amount of the thermolabile  $\alpha$ -amylase.



**Figure 2.** Formation of mnm<sup>5</sup>s<sup>2</sup>U

also found that MnmA had the ATP hydrolysis activity and that ATP protected MnmA from trypsinolysis, suggesting the presence of an ATP-binding site in MnmA. These results indicated that MnmA and IscS catalyze the synthesis of s<sup>2</sup>U in tRNA by using ATP and L-cysteine.

March 2006.

Kurihara T, Production of useful compounds and bioremediation of environments by cryobiotechnology using cold-adapted microorganisms, (NEDO), 1 April 2001 - 31 March 2004.

Kurihara T, In vivo and in vitro analysis of selenium metabolism - a multidisciplinary approach, Cooperative Research under the Japan-U.S. Cooperative Science Program (JSPS) 1 April 2001 - 31 March 2004.

# **Molecular Biology and Information**- Biopolymer Structure -

http://www.kuicr.kyoto-u.ac.jp/labos/mbi1/scope\_J.html



Prof UMEDA, Masato (D Pharm Sc)



Instr TAKEUCHI, Ken-ichi (D Pharm Sc)



Instr KATO, Utako (D Sc)

## **Student**TANIUCHI, Kentaro (M1)

### Scope of Research

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

- (1) Identification of a series of proteins that regulate molecular motion of lipid molecules and elucidation of their role in cellular and animal morphogenesis.
- (2) Establishment of a series of Drosophila mutants with aberrant temperature preference (*atsugari*, *samugari*, etc) and elucidation of the molecular relationship between the temperature-responding membrane systems and animal behaviors.

### **Research Activities (Year 2003)**

### **Presentations**

Transbilayer lipid movements: A role in cell division and cell polarity formation. Umeda M. Gordon Research Conference on Molecular and Cellular Biology of Lipids, 20-25 July, Meriden, NH. USA.

Identification of Ros3p, a novel membrane protein required for phospholipid translocation across the plasma membrane in Saccharomyces cerevisiae. Kato U., Emoto K., Umeda M. Gordon Research Conference on Molecular and Cellular Biology of Lipids, 20 - 25 July, Meriden, NH. USA.

Membrane lipid control of Cytokinesis. Umeda M., Emoto K., Kato U. Symposium on A break-through in researches on functional glycerolipids. The 76th Annual Meeting of the Japanese Biochemical Society. 15 - 18 October, Yokohama.

Regulation of membrane phospholipid dynamics and its role in cell polarization. Kato U., Umeda M. Symposium on dynamics of the intracellular molecular networks. The 76th Annual Meeting of the Japanese Biochemical Society. 15 - 18 October, Yokohama.

Lipid Analisis in *Drosophila* cryophilic mutant, *atsug-ari*, Takeuchi T., Umeda M., *et al*. The 76th Annual Meet-

ing of the Japanese Biochemical Society. 15 - 18 October, Yokohama.

Local change in membrane lipid composition during cytokinesis. Umeda M. The 25th Symposium on Biomembrane-Drug Interaction of the Pharmaceutical Society, 13 - 14 November, Kanazawa.

Development of phospholipid-specific probes and their application to cell biology. Umeda M. Symposium of Japanese Consociation for Phosphatidylserine. 21 November, Tokyo.

### **Grants**

Umeda M., Cellular morphogenesis based on the positional information of membrane phospholipids. Grantin-Aid for Scientific Research (A)(2), 1 April 2003 - 31 March 2006.

Umeda M., Identification of genes involved in thermoregulatory 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 2005.

## Regulation of membrane phospholipid dynamics and its role in cell polarity formation

Polarity formation is important for biological phenomena such as cell morphogenesis, movement, proliferation and organism development. Although recent studies have revealed that cytoskeletal and membrane systems participate in this process, it is unclear how they cooperate with each other. We have identified a novel membrane protein, Ros3p, that is required for the transbilayer movement (flipflop) of phospholipids across the yeast plasma membrane (Fig.1). Ros3p deficient cells exhibited abnormal morphology (Fig.2b) and disorganized cortical actin patches. Overproduction of Ros3p caused multibudded cells (Fig.2c). These results suggest that Ros3p is involved in both the regulation of phospholipid movement and the actin organization in yeast.

Ros3p is highly conserved among various organisms including worm, fly and mammals. In mammalian cells, overproduction of Ros3p also resulted in multinucleus. Moreover, mouse homolog is localized at the apical side of the epithelial tissues, implying a role of Ros3p in polarized vesicular transport. We propose that Ros3p may function as a coordinator between membrane phospholipids organization and cell polarization via polarized vesicular transport.

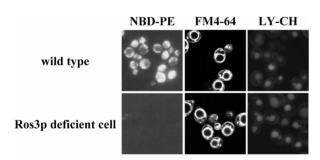


Fig. 1 Internalization of fluorescence-labeled phospholipid and endocytic markers.

In Ros3p deficient cells, the uptake of fluorescence-labeled phosphatidylethanolamine (NBD-PE) was markedly decreased but endocytic markers (FM4-64 and LY-CH; a lipophilic or soluble dye respectively) were not affected.

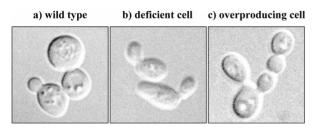


Fig. 2 Abnormal morphology of Ros3p -deficient or -overproducing cells

## Defective expression of a *Drosophila* homologue of dystroglycan in a cryophilic mutant, atsugari

Behavior plays a major role in thermoregulation in both ectothermic and endothermic species. A wide variety of animals has been shown to move towards and remain preferentially in a thermally comfortable environment. Moreover the preferred temperature differs among species as well as among individuals within a species. Progress has been made in the identification of molecules involved in the sensation of peripheral temperature, but molecular mechanisms underlying temperature preference remain poorly understood. In an effort to identify genes involved in behavioral thermoregulation, we searched for mutations that affect temperature preference of Drosophila melanogaster. We identified a new Drosophila mutant with a preference for unusually low temperatures and we designated the mutant atsugari (Fig. 3). We found that the atsugari phenotype was caused by the reduced expression of the Drosophila homologue of dystroglycan (DmDG; Fig 4), a membrane glycoprotein that forms the core of the dystrophin-glycoprotein complex. Reduced expression of DmDG induced a significant increase in the fluidity of membrane lipids that was associated with the cryophilic phenotype. Our studies demonstrate a novel role for dystroglycan in thermoregulation of Drosophila. The atsugari mutant provides a unique model for studies of the physiological functions of dystroglycan.

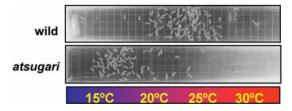


Fig. 3 Representative results of temperature-preference assays. Third-instar wandering larvae were placed on a linear thermal gradient and the distribution of the larvae after 20 min of wandering was recorded.

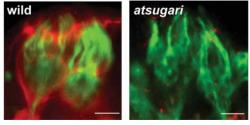


Fig. 4 Patterns of expression of DmDG in embryonic neural tissues. Sensory organs in the wild type and the *atsugari* mutant were immunostained with DmDG-spscific antibodies (red) and neuron-specific monoclonal antibody (green). Scale bars: 10 mm

# **Molecular Biology and Information**- Molecular Biology -

### http://molbio.dyndns.org/



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### **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 cellualr proteins in higher plants and pathogens. The major subjects are mechanisms involved in intracellular signal transduction and regulation of gene expression responsive to environmental stimuli, differentiation and development of plant organs, and plant-microbe interaction. As of December 2003, study is being concentrated on the roles of two-component response regulators involved in cytokinin signaling for cell growth and division and of homeodomain proteins modulating phospholipid signaling for root-hair development.

### **Research Activities (Year 2003)**

### **Presentations**

Analysis of function of CDKA expressed in Arabidopsis trichome, Imai K, Ohashi Y, Aoyama T, Oka A, 2003 Ann Meeting (Nara) of Jpn Soc Plant Physiol, 27 - 29 March (Osaka).

GLABRA2 regulates root-hair development by modulating phospholipid signaling, Ohashi Y, Oka A, Pousada R, Possenti M, Ruberti I, Morelli G, Aoyama T, VII International Congress of Plant Molecular Biology, 23 - 28 June (Barcelona, Spain),

Cytokinin signaling and two-component regulatory system, Oka A, Gamma Field Symposia No.42 (Institute of Radiation Breeding, NIAR MAFF) 'Molecular mechanisms of and mutations in plant hormone responses and signal transduction', 16 - 17 July (Mito).

Function of phospholipase D in root-hair development, Aoyama T, 16th Plant Lipid Symposium, 28 - 29 November (Yamaguchi).

Interactions between plant transcription factors and their target genes, Aoyama T, Taniguchi M, Ohashi Y, Oka A;

Functinal analysis of A2 cyclins expressed in Arabidopsis trichome cells, Imai K, Ohashi Y, Aoyama T, Oka A, 2003 Ann Meeting of Mol Biol Soc Jpn, 10 - 13 December 2003 (Kobe).

### **Grants**

Oka A and Aoyama T, Molecular basis of cytokinin signaling in plant cells, Grant-in-Aid for Scientific Research on Priority Areas (A), 1 April 2003 - 31 March 2005.

Aoyama T and Oka A, Molecular mechanism of adaptive responses controlled by *Arabidopsis* His-Asp phosphorelay signal transduction, Grant-in-Aid for Scientific Research on Priority Areas (B), 1 April 2000 - 31 March 2005.

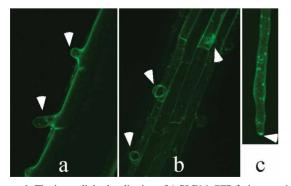
### Award

Ohashi Y, The ICR Award for Young Scientists, Functinal analysis of the *Arabidopsis GLABRA2* gene that contributes root-hair development through the modulation of phospholipid signaling, ICR, 5 December 2003.

## Phospholipid signaling modulated by GLA-BRA2 contributes root-hair development

Cell morphogenesis and its disposition pattern are crucial for plants to ensure functional tissue and organ structures because the relative positions of plant cells do not change after proliferation. The Arabidopsis root epidermis is composed of two types of cell files, only one of which produces root hairs. Each hair cell file makes contact with two adjacent underlying cortical cell files, whereas each hairless cell file makes contact with a single cortical cell file. Mutations in the GLABRA2 (GL2), WEREWOLF (WER), and TRANSPARENT TESTA GLABRA 1 (TTG1) genes lead to the generation of root hairs from all the cell files. Conversely, mutations in CAPRICE (CPC) reduce the frequency of root hairs in hair cell files. The homeodomain protein GL2 is synthesized predominantly in hairless cell files. TTG1 positively controls GL2 expression. The Myb-type transcription factors WER and CPC, which cross-control each other in a feedback loop, positively and negatively regulate the position-specific expression of GL2, respectively. Thus a transcriptional regulatory circuit appears to be involved in determining root-hair pattern formation. We have now analyzed their downstream events by identifying genes targeted by GL2 [1], the transcription factor farthest downstream in the known feedback loop.

We conducted a subtraction experiment using cDNAs prepared from plants synthesizing a modified version of GL2 (constitutively active for transactivation) and the native GL2 (repressor) to detect GL2-target genes that promote root-hair development. One of such genes encoded a phospholipase D (PLD) named AtPLD $\zeta$ 1. GL2 bound to a promoter region of  $AtPLD\zeta$ 1. Furthermore,  $AtPLD\zeta$ 1 expression in developing wild-type root epidermis was higher in hair cell files than in hairless cell files. In contrast, mutations in GL2 as well as in the GL2-binding region upstream of  $AtPLD\zeta$ 1 abolished this expression specificity by elevating transcription levels in hairless cell files. It was thus concluded that GL2 works as a repressor for the  $AtPLD\zeta$ 1 gene.



**Figure 1.** The intracellular localization of AtPLDζ1-GFP fusion protein, visualized by its autofluorescence under a confocal laser-scanning microscope. The arrowheads indicate relatively strong fluorescence signals around bulges (a, b) and the root-hair apex (c). Quoted from ref 1.

AtPLD\(\xi\)1 (a fusion derivative with green fluorescent protein GFP) was localized in vesicles mainly at the cell cortical region (Figure 1). At early stages of root-hair development, the fusion protein was localized preferentially around bulges (Figure 1a, b). In growing root hairs, relatively strong fluorescence was often observed around the root-hair apex (Figure 1c). Both elevation and reduction of AtPLDζ1 expression led to various abnormalities in roothair development. PLD hydrolyzes phosphatidylcholine to generate phosphatidic acid and choline. Arabidopsis encodes two types of PLDs, plant-specific type and universal type for eukaryotes. AtPLDζ1 is of the latter type. The universal type PLDs in animal and yeast cells modulate membrane-trafficking events to and from the plasma membrane. By analogy, AtPLD\(\zeta\)1 might regulate vesicle trafficking and exocytosis in root-hair tip growth. The localization pattern of the GFP-fusion protein supports this postulate.

1. Ohashi, Y. et al. Science, 300, 1427-1430 (2003).

### Genes encoding enzymes involved in protocatechuate *meta*-degradation pathway of *Pseudomonas ochraceae*

Protocatechuate (PCA) is a common intermediate in the biodegradation of various aromatic compounds including phthalate, fluorene, and various methoxy derivatives of benzoate. Some microorganisms e.g. ligninassimilating Sphingomonas paucimobilis and phthalateassimilating Arthrobacter keyseri, metabolize PCA through *meta*-degradation pathway ( $\alpha$ -keto acid pathway), in which PCA undergoes the 4,5-cleavage by PCA 4,5-dioxygenase to give 4-carboxy-2-hydroxymuconate-6-semialdehyde (CHMS). CHMS is then converted to 2-pyrone-4,6-dicarboxylate (PDC) by NAD(P)<sup>+</sup>-dependent CHMS dehydrogenase. PDC is hydrolyzed by PDC lactonase to give 4-ozalomesaconate, which is hydrated by 4-oxalomesaconate hydratase, and finally cleaved to pyruvate and oxaloacetate by 4-hydroxy-4-methyl-2-oxoglutarate aldolase [2]. The molecular mechanism of each enzyme-catalyzed reaction is hampered owning to the deficient information of the enzyme structure and the lack of an over-expression system of the enzyme.

A 7.5-kb *EcoRI* DNA fragment from the *P. ochraceae* NGJ1 chromosome was previously shown to carry a promoter-like sequence and genes encoding transporter, 4-oxalomesaconate hydratase, 4-hydroxy-4-methyl-2-oxoglutarate aldolase, and 3'-truncated PDC lactonase. To elucidate the whole genetic structure corresponding to enzymes involved in the pathway, a DNA fragment downstream of the *EcoRI* fragment was cloned. As a result, this region corresponded to the  $\alpha$  and  $\beta$  subunits of PCA 4,5-dioxygenase, CHMS dehydrogenase, and the 3'-half of PDC lactonase. These enzymes were excessively synthesized in *E. coli* cells, and purified to homogeneity through several steps of chromatography. Their molecular and catalytic properties were found to be indistinguishable from those isolated from *P. ochraceae* cells.

2. Maruyama, K. et al. Biosci. Biotech. Biochem. 65, 2701-2709 (2001).

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

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Res LI, Yongming (D Sc)

### **Students**

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### **Visitor**

BESSON, Eric

Univeriste de Montpellier II, France, 2 July 2003 - 20 August 2003

### Scope of Research

Our research is concerned with some new aspects in the elemento-organic chemistry, including (1) the design and synthesis of novel  $\pi$ -conjugated systems containing main group elements such as boron and silicon for electronic and photonic applications, (2) the synthesis, structural studies, and synthetic applications of organosilicon compounds, such as pentacoordinate silicon compounds and functionalized silyl anions, (3) the elucidation of the  $\sigma$ -conjugation in the polysilane framework using the configuration-constrained oligosilane model systems, (4) the old but new chemistry of the disilapropellane and related compounds, and (5) the development of new efficient reactions using main group element reagents and transition metal complex catalysts.

### Research Activities (Year 2003)

### **Presentations**

Elements Science: Elemento-Organic Chemistry directed toward Materials Science (Plenary lecture), Tamao K, The International Symposium on Dynamic Complexes. 4 August, Tokyo, Japan.

Silole-Containing pi- and sigma-Conjugated Polymers, Tamao K, The Third International Workshop on Silicon-Containing Polymers, 23 - 24 June, Troy, New York, USA.

Organosilicon Chemistry, Cross-Coupling Reaction, and Fruitful Blend with Each Other, Tamao K, The Noyori Forum, 20 - 21 September, Kanagawa, Japan.

Elements Science: Organo Main Group Chemistry directed toward Materials Science, Tamao K, Synthetic Organic Chemistry Workshop, Society of Synthetic Organic Chemistry, Japan, 5 - 6 November, Tokyo, Japan.

Relationship between Structure and Photophysical Properties of Disilanes, Tsuji H, Casher DL, Kubota M, Kobayashi T, Toshimitsu A, Michl J, Tamao K, 50th Symposium on Organometaiilc Chemistry, 30 September, Osaka, Japan.

### **Grants**

Tamao K, Elements Scienece towards Construction of Organic and Inorganic Frameworks Focusing on Quality of Elements, Grant-in-Aid for Scientific Research on COE, April 2000 - March 2005.

Tsuji H, Development of new method of controlling silicon chain conformation aiming at controlling photophysical properties of oligosilanes, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.

Tsuji H, Construction of new conjugation system containing polysilane and porphyrin, Grant-in-Aid on Priority Areas, 1 April 2003 - 31 March 2004.

### **Awards**

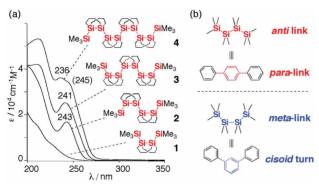
Tamao K, The Asahi Prize, Development of Innovative Organometallic Reactions, Asahi Culture Foundation, 31 January.

Tamao K, The 14th Mukai Prize, Discovery of Cross-Coupling Reaction and Its Application, Tokyo Ohka Foundation for Promotion of Science and Technology, 5 June.

## σσ\* Transition in anti,cisoid-Alternating Oligosilanes up to Docosasilane (Si<sub>22</sub>)

The photophysical properties of polysilane  $\sigma$ -conjugated system are sensitive to the silicon backbone conformation. So far, we have demonstrated the conformation dependence on the basis of UV absorption spectra of conformationally constrained tetra- and hexasilanes, which claims that an *anti* link (SiSiSiSi dihedral angle  $\omega \sim 180^\circ$ ) effectively extends the  $\sigma$ -conjugated system while a *syn* turn ( $\omega$  < ca. 30°) at the termini does not [1]. For a better understanding of the electronic states and photophysical properties in polysilanes, we have extended the investigation to longer silicon chain compounds.

As shown in Figure 1a, on the basis of the UV absorption spectra of the *anti,cisoid*-alternating oligosilanes **2-4**, experimental clear-cut evidence is presented for the generally accepted idea that the  $\sigma$  conjugation in polysilanes does not effectively extend through a tetrasilane fragment with a small dihedral angle such as a *cisoid* turn ( $\omega \sim 30^{\circ}$ ) [2], which was confirmed to be the case with longer *anti,cisoid*-alternating oligosilanes up to Si<sub>22</sub> [3].



**Figure 1.** (a) UV absorption spectra of the *anti,cisoid*-alternating oligosilanes **1-4**; (b) comparison between σ- and π- conjugation systems.

The UV absorption of all-transoid permethylated oligosilanes and the anti, cisoid-alternating oligosilanes is similar to that of  $\pi$ -conjugated poly(p-phenylene)s and poly(m-phenylene)s, respectively (Figure 1b). Thus, the effect of the conformation isomerism on the photophysical properties in the  $\sigma$ -conjugation systems corresponds to that of the position isomerism in the  $\pi$ -conjugated systems.

- 1. Tsuji H, Michl J, Tamao K J. Organomet. Chem., 685, 9-14 (2003).
- Tsuji H, Terada M, Toshimitsu A,Tamao K J. Am. Chem. Soc., 125, 7486-7487 (2003).
- 3. Honnaiah M, Tsuji H, Tamao K, submitted for publication.

### Lewis Acid Induced Palladium Catalyzed Cross-Coupling Reaction of 1-Aryltriazene with Areneboronic Acids

Nickel or palladium-catalyzed cross-coupling reaction utilizing organic halides and a variety of organometallic reagents has become one of the most powerful synthetic tool for the formation of carbon-carbon and carbon-heteroatom bond. We have recently developed the cross-coupling reaction of 1-aryltriazenes, instead of organic halides, as an electrophile with organometallic reagents such as areneboronic acids and aryltrifluorosilanes. The cross-coupling reaction of 1-(*p*-tolyl)triazene with *p*-anisylboronic acid proceeds smoothly in the presence of a catalytic amount of palladium catalyst and phosphine ligand together with 1 equiv. of boron trifluoride (Scheme 1). The addition

Scheme 1. Cross-coupling reaction of 1-aryltriazene with areneboronic acid.

of boron trifluoride is essential for the formation of biaryl product; no reaction occurs at all without Lewis acid. The reaction proceeds quickly even at room temperature to afford the desired product in high yield.

While the reaction mechanism is not clear at the present time, it is supposed that the boron trifluoride plays two roles in the reaction process; (1) the boron trifluoride first serves as a Lewis acid toward the 1-aryltriazene to enhance the reactivity of  $sp^2$ -carbon–nitrogen bond and (2) the resulting borate moiety serves as a fluoride base to promote a transmetallation of the areneboronic acid.

**Scheme 2.** Cross-coupling reaction of 1-aryltriazene with aryltrifluorosilane.

A similar cross-coupling reaction of 1-aryltriazene with aryltrifluorosilanes has also been achieved without a Lewis acid, although the increased amount of catalyst and prolonged reaction time are necessary (Scheme 2). It is supposed that the Lewis acidic triflurosilane itself serves as a Lewis acid to enhance the reactivity of the triazene component.

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

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### **Scope of Research**

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

- High- $T_c$  superconducting copper oxides with higher  $T_c$  or  $J_c$ .
- Perovskite-based compounds with unusual magnetic and electronic properties.
- Low-dimensional spin system showing dramatic quantum effects.

### Research Activities (Year 2003)

### **Presentations**

Ligand Holes: SrFeO<sub>3</sub> and (Ca,Na)<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub>, Takano M, International Workshop on Strongly Correlated Transition Metal Compounds, 4 - 7, August.

High Pressure Synthesis and Crystal Structure of Perovskite BiNiO<sub>3</sub> and Effects of A-Site Substitution, Ishiwata S, Azuma M, Kato K, Nishibori E, Vacate M, Skated M, Takano M, Joint 19th AIRAPT-41st EHPRG International Conference on High Pressure Science and Technology, 7 - 11, August.

High-pressure Synthesis and Physical Properties of Bi-

Contained Transition Metal Oxides BiCrO<sub>3</sub>, and BiCoO<sub>3</sub>, Niitaka S, Azuma M, Takano M, Nishibori E, Takata M, Sakata M, Joint 19th AIRAPT-41st EHPRG International Conference on High Pressure Science and Technology, 7 -11, August.

Single Crustal Growth of PrNiO<sub>3</sub> Perovskite at 4.5 GPa and the Study of its Metal-Insulator Transition, Saito T, Azuma M, Nishibori E, Takata M, Sakata M, Nakayama N, Arima T, Kimura T, Urano C, Takano M, Joint 19th AIRAPT-41st EHPRG International Conference on High Pressure Science and Technology, 7 - 11, August.

### Blue-Light Emission from SrTiO<sub>3</sub>

Blue-light emission was observed from SrTiO<sub>3</sub> single crystal with oxygen deficiencies caused by Ar<sup>+</sup> ion beam irradiation. Emission intensity increased with the increase of Ar<sup>+</sup> irradiation time. New electronic state (E=2.8eV) is generated by the Ar<sup>+</sup> irradiation. Light emission of SrTiO<sub>3</sub> might be caused by the excitonic mechanism. Light emission devices with short wave length and high power using Ti<sup>3+</sup> containing perovskite are expected in the future.



Figure 1. Cathode luminescence of SrTiO<sub>3</sub>.

### **Cubic FePt nanoparticles**

Colloidal nanoparticles are promising candidates in a wide range of technological applications and have been the subject of numerous works. Although synthetic works have focused on the preparation of monodisperse spherical nanoparticles with a controlled size, physical and chemical properties are mostly dependent not only on size but also on shape. We have succeeded in synthesizing monodisperse FePt nanoparticles with a *cubic* shape for the first time based on a simple organic-phase reaction. 2-D array of the present cubic nanoparticles can be a promising candidate for a "bit per particle" data storage media.

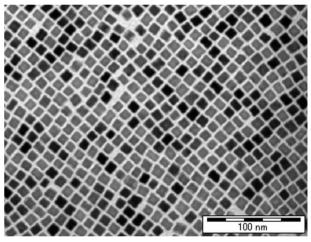


Figure 2. FePt nanoparticles with a cubic shape.

### Grants

Takano M, Development of 3d transition-metal oxides with oxygen p holes. Grant-in-Aid for Scientific Research (A) (2), 1 April 2002 - 31 March 2005.

Terashima T, Electric field induced superconductivity in the FET devices using ultrathin SrTiO<sub>3</sub> single-crystal substrate with high dielectric constant. Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2004.

Terashima T, Preparation and properties of epitaxial thin films of oxides containing transition-metal ions in unusually high-valence states, Priority Area Grants from the Ministry of Education, Science, Culture and Sport of Japan, 1 April 2000 - 31 March 2004.

Azuma M, Exploration of photo-functions in strongly correlated electron systems of transition metal oxides, PRESTO, 1 December 2001 - 31 November 2004.

### **Awards**

Takano M, 2002 JSPM Award for Distinguished Achievements in Research, Discovery of Novel 3d-Transition Metal Oxide: High-Pressure Synthesis, The Japan Society of Powder and Powder Metallurgy, 21 May 2003.

Ishiwata S, The ICR Award for Students, High Pressure Synthesis and Crystal Structure of Perovskite BiNiO<sub>3</sub>, and Suppression of A-site Charge Disproportionation by Lasubstitution, ICR, 5 December 2003.

### **International Research Center for Elements Science**

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### Scope of Research

This is a new research laboratory launched in the 2003 academic year, aiming 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) synthesis and catalytic properties of transition metal—heavy element complexes, and (3) development of highly efficient ways of constructing functional organic molecules.

### Research Activities (Year 2003)

### **Presentations**

Convenient Route to Thio- and Selenocarbene Ruthenium Complexes Serving as Highly Selective Catalysts for Ring-Opening/Cross Metathesis, Katayama H, Nagao M, Ozawa F, The 15th International Symposium on Olefin Metathesis and Related Chemistry (ISOM XV), 28 July - 1 August, Kyoto, Japan.

Synthesis, Structure, and Alkyne Insertion Reactions of Platinum–Group 14 Element Complexes, Sagawa T, Ozawa F, 92nd CATSJ Meeting, 18 - 21 September, Tokushima, Japan.

Synthesis of Unsymmetrically End-Functionalized Poly(norbornene)s by Ring-Opening Metathesis Polymerization/Chain-Transfer System, Katayama H, Ozawa F, *et al.*, SPSJ 52nd Symposium on Macromolecules, 24 - 26 September, Yamaguchi, Japan.

Synthesis and Reactions of Hydridoplatinum(II) Complexes Bearing Diphosphinidenecyclobutene Ligands (DPCB), Ishiyama T, Ozawa F, *et al.*, 50th Symposium on Organometallic Chemistry, Japan, 28 - 30 September, Osaka, Japan.

Development of Highly Selective Catalysis for the Synthesis of Tailored Polymers, Ozawa F, Katayama H, et al.,

JPI Symposium 2003 in Osaka, 17 - 19 November, Osaka, Japan.

Highly Reactive Organometallic Complexes Bearing Diphosphinidenecyclobutene Ligands: Synthesis and Catalysis, CSJ Hiroshima Seminor, 6 December, Higashihiroshima, Japan.

### **Grants**

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

Ozawa F, Development of Novel Catalysis using 5-Membered Chelate Complexes with sp<sup>2</sup>-Hybridized Phosphorus Atoms, Grant-in-Aid for Scientific Research on Priority Areas, Apr. 2002 - Mar. 2004.

Ozawa F, Novel Organometallic Complexes with Phosphaalkene Ligands: Synthesis and Catalysis, Grand-in-Aid for Scientific Research (B) (2), Apr. 2003 - Mar. 2006.

Katayama H, Stereocontrolled Synthesis of  $\pi$ -Conjugated Polymers Using Transition Metal Catalysts, The Ogasawara Foundation for the Promotion of Science & Engineering, Apr. 2003 - Mar. 2004.

### (π-Allyl)palladium Complexes Bearing Diphosphinidenecyclobutene Ligands (DPCB): Highly Active Catalysts for Direct Conversion of Allylic Alcohols

sp²-Hybridized phosphorus compounds have a marked tendency to engage in metal-to-phosphorus  $\pi$ -backbonding and have a strong  $\pi$ -acceptor property comparable to that of the carbonyl ligand. Therefore, unlike common phosphine and cyclopentadienyl ligands, DPCB may effectively enhance the electrophilicity of metal centers. We have found in this study that ( $\pi$ -allyl)palladium complex (1) bearing DPCB ligands effectively catalyze the direct allylation of aniline and active methylene compounds with allylic alcohols [1]. These reactions proceed via a novel allylation mechanism including a hydridopalladium intermediate, which is significantly acidic due to the unique coordination property of DPCB ligand.

R
OH + NuH
$$\frac{\text{Mes}^*}{-H_2\text{O}}$$
NuH = PhNH<sub>2</sub>, CH<sub>2</sub>(CO<sub>2</sub>Et)<sub>2</sub>, etc

Scheme 1. Direct conversion of allylic alcohols catalyzed by (DPCB)-Pd( $\pi$ -allyl) complex 1.

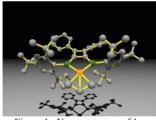


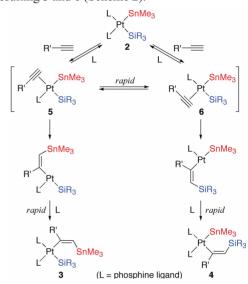
Figure 1. X-ray structure of 1.

1. Ozawa F, Okamoto H, Kawagishi S, Yamamoto S, Minami T, Yoshifuji M, J. Am. Chem. Soc., 2002, 124, 10968.

## Alkyne Insertion into cis-Silyl(stannyl)-platinum(II) Complexes

Addition of inter-element linkages to alkynes catalyzed by group 10 metal complexes has attracted a great deal of recent interest. We have elucidated the mechanism of alkyne insertion into *cis*-silyl(stannyl)platinum complexes (2), which are models of key intermediates for palladium-catalyzed silylstannylation of unsaturated hydrocarbons [2]. Complexes 2 undergo competitive insertion of alkynes into the Pt–Sn and Pt–Si bonds. The ratio of the resulting insertion complexes 3 to 4 is significantly affected by the types of silyl and phosphine ligands and alkynes employed. The variations thus observed have been reason-

ably interpreted on the basis of the insertion mechanism involving associative displacement of one of the phosphine ligands in 2 with alkynes, followed by competitive migration of the stannyl and silyl ligands on the alkyne ligand in the resulting 5 and 6 (Scheme 2).

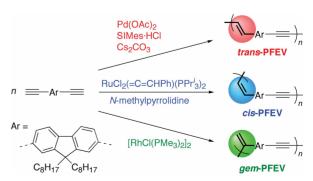


**Scheme 2.** Mechanism of alkyne insertion into *cis*-silyl(stannyl)platinum(II) complexes **2**.

2. Sagawa T, Sakamoto Y, Tanaka R, Katayama H, Ozawa F, *Organometallics*, **2003**, *22*, 4433.

### Polyaddition of 2,7-Diethynyl-9,9-dioctyl fluorene Using Regio- and Stereoselective Alkyne-Dimerization Catalysts

We have succeeded in regio- and stereocontrolled synthesis of poly(fluorene ethynylene vinylene)s using catalytic polyaddition process (Scheme 3). The structure of vinylene units clearly reflects the nature of catalysts observed in the prototype dimerization reactions of arylacetylenes. These polymers show marked differences in optical properties dependent on the structure of the main chain [3].



**Scheme 3.** Regio- and stereocontrolled synthesis of PFEVs.

3. Katayama H, Nakayama M, Nakano T, Wada C, Akamatsu K, Ozawa F, *Macromolecules*, in press.

## **Bioinformatics Center** - Bioknowledge Systems -

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



Prof KANEHISA, Minoru (D Sc)



Assoc Prof GOTO, Susumu (D Eng)



Instr KAWASHIMA, Shuichi



Vis Instr HATTORI, Masahiro



PD KAWANO, Shin (D Eng)



PD SCHWARTZ, Jean-Marc (D Eng)



PERRET, Jean-Luc (D Sc)



JAUREGUI, Ruy (D Sc)

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HONDA, Wataru OH, Min-A

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OKUDA, Shujiro (D1) YAMADA, Takuji (D1) SAKIYAMA, Tadahiko (M2) SASAKI, Naobumi (M2) SATO, Tetsuya (M2) MIYAMA, Takashi (M1) OTA, Koji (M1)

### Scope of Research

Owing to continuous developments of high throughput experimental technologies, ever increasing amounts of data are being generated in genomics and proteomics. We have been developing bioinformatics technologies for analyzing a large number of genes or proteins at a time, toward the understanding and utilization of higher order functional bihaviors of the cell or the organism. The suite of databases and associated software that we develop is called KEGG and is made publicly available as part of the GenomeNet service (http://www.genome.jp).

### Research Activities (Year 2003)

### **Grants**

Kanehisa M, Biological systems database (KEGG) and genome information science. Research for the Future Program, JSPS.

Kanehisa M, BRITE: deductive database of the genome and the biological system based on binary relations. Bioinformatics Research and Development, JST.

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

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

Kanehisa M, Development of the integrated database for bacterial genomes and their cellular function. Grantin-Aid for Scientific Research on Priority Areas "Genome Biology", MEXT.

Goto S, Construction and retrieval of highly integrated biological databases. Grant-in-Aid for Scientific Research on Priority Areas "Genome Information Science", MEXT.

## **KEGG Orthology : a hierarchical classification** of all functional orthologs in gene universe

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

Using KEGG/SSDB database, we classify and annotate orthologs both automatically and manually. Namely, orthologs are classified by a computational clustering method according to the KEGG/SSDB scores (Fig. 1), and the function of each ortholog is further examined manually. In order to support this annotation process, GFIT(Gene Function Identification Tool) program is developed and is now available on WWW (Fig. 2).

## Chemical Ontology: a systematic classification of all biochemical objects in chemical universe

Chemical Ontology is a new on-going project to define and classify chemical functionality among all chemical objects, that is, chemical compounds and enzymatic reactions observed in any biological process.

To achieve this end, we first define the similarity measure of chemical compounds on the basis of the graph comprison method, and then classify all of metabolites into several hundreds of clusters. With these results, we can make a clear view of relationship between chemical universe and genomic contexts, here, operon-like structures of genes (Fig. 3).

As for enzymatic reactions, we are now trying to develop a novel classification scheme mainly based on another structural comparison method. We have been in difficulties with the traditional EC numbering, however, with our new classification policy we are expected to perform more reasonable analyses in biological pathways. For instance, Fig. 4 is one of tentative results that we have already demonstrated with a premature version of our system.



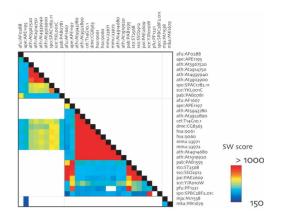


Fig. 1 All genes are clustered on the KEGG/SSDB scores.

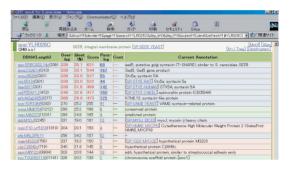
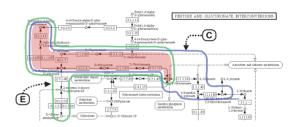


Fig. 2 GFIT is a supporting tool for the annotation of gene.



**Fig. 3** Some of chemical compound clusters are highly correlated with operon-like structures in genomes.

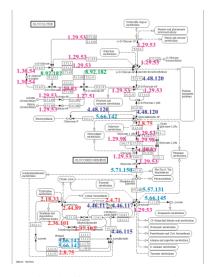


Fig. 4 Our reaction classification can detect reaction modules.

## **Bioinformatics Center** - Biological Information Network -

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



Prof AKUTSU, Tatsuya (D Eng)



Instr UEDA, Nobuhisa (D Eng)



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FUKAGAWA, Daiji (D1) MOESA, Harry Amri (M2)

### Visitors

Prof HALLDORSON, Magnus University of Iceland, 21 April, 2003

Ecole des Mines de Paris, 24 October - 8 November, 2003 Dr VERT, Jean-Philippe Mr CUTURI, Marco Ecole des Mines de Paris, 27 October - 31 October, 2003 Mr MAHE, Pierre Ecole des Mines de Paris, 1 December - 12 December, 2003

### Scope of Research

Due to rapid progress of the genome projects, whole genome sequences of many organisms and a draft of human genome sequence have been already determined. But, the determination of the whole genome sequences does not mean the end of analysis of genetic code. In order to understand the meaning behind the genetic code, we have been developing algorithms for analyzing proteomics data and genomics data. Recently, we focus on the following topics: protein-protein interaction, remote homology detection, and cheminformatics.

### Research Activities (Year 2003)

### **Presentations**

Efficient extraction of mapping rules of atoms from enzymatic reaction data, Akutsu T, The 7th Annual Int'l Conf. on Research in Computational Molecular Biology, 12 April.

Optimization problems and metaheuristics in bioinformatics, Akutsu T, The 5th metaheuristics Int'l Conf., 28 August.

Performance analysis of a greedy algorithm for inferring Boolean functions, Fukagawa D, Akutsu T, The 6th Int'l Conf. on Discovery Science, 18 October.

Inferring strengths of protein-protein interactions from experimental data using linear programming, Hayashida M, Ueda N, Akutsu T, European Conf. on Computational Biology, 28 September.

Computational and statistical methods in bio-informatics, Akutsu T, The 14th Int'l Symp. Methodologies for Intelligent Systems, 28 October.

### **Grants**

Akutsu T, Miyano S, Ueda N, Algorithms for finding common patterns in bioinformatics, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2005.

Akutsu T, Genome information science (a member of the project), Grant-in-Aid for Scientific Research Priority Areas (C), 1 April 2000 - 31 March 2005.

Ueda N, Statistical language models that generate a pair of sequences for sequence analysis, Grand-in-Aid for Encouragement of Young Scientists, 1 April 2003 - 31 March 2006.

## Inferring strengths of protein-protein interactions with linear programming

Since protein-protein interaction plays a key role in any cellular processes, several computational methods have been proposed for inference of protein-protein interaction. They consider that the interaction is represented as binary, i.e., whether two proteins interact or not. However a data set of the ratios (strengths) of interaction between two proteins becomes available since multiple experiments of the interactions for the same protein pairs were performed recently in practice. We then develop a new method to infer the strength of the interaction with linear programming. Experimental results show that it outperforms existing methods on the data set of the ratios of interactions.

1. Hayashida M, Ueda N, Akutsu T, Inferring strengths of protein-protein interactions from experimental data using linear programming, Bioinformatics, 19, supplement, pp. ii58 - ii65 (2003).

## Efficient extraction of mapping rules of atoms from enzymatic reaction data

Extraction of mapping rules of atoms from enzymatic reactions is useful for drug design, simulation of tracer experiments and consistency checking of pathway databases. Most of previous methods for this problem are based on maximal common subgraph algorithms. We then propose a novel approach based on graph partition and graph isomorphism. The results of computational experiments suggest that the proposed method is useful in many cases.

 Akutsu T, Efficient extraction of mapping rules of atoms from enzymatic reaction data, 7th Annual Int'l Conf. on Research in Computational Molecular Biology, pp. 1 - 8 (2003).

## Protein homology detection using string alignment kernels

Several methods have been developed recently for remote homology detection for protein sequences using support vector machines (SVMs), and we developed one method called SVM-SW. To achieve higher accuracy of the detection, we improved the method by designing a new kernel function which measures similarity between two protein sequences with the local alignment. The designed kernel function and SVMs (Fig. 2) performed better than several existing methods on a benchmark data set.

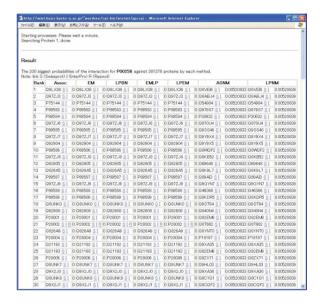


Figure 1. A system for inferring strengths of protein-protein interac-



**Figure 2.** A system for protein remote homology detection using string kernels.

# **Bioinformatics Center**- Pathway Engineering -



Prof MIYANO, Satoru\* (D Sc) [Adjunct Prof]

### Scope of Research

This laborabory develops research on computational knowledge discovery, e.g. inference of pathway information from gene expression profile data, and simulation system for cells and organisms through the biopathway simulation of gene regulatory networks, signaling pathways, metabolic pathways, and physical simulations, etc. With this approach, the functions of genes and systems of genes will be analyzed and predicted.

### Research Activities (Year 2003)

### **Presentations**

Gene Networks: Inference, Modeling and Simulation, Miyano S, Seminar on Functional Genomics, AAAS Annual Meeting and Science 2003, Denver, USA, 16 February 2003.

Estimating gene networks from gene expression data by combining Bayesian network model with promoter element detection, Tamada Y, Kim S, Bannai H, Imoto S, Tashiro K, Kuhara S, Miyano S, European Conference on Computational Biology 2003, Paris, France, 27-30, September 2003.

Inference, Modeling and Simulation of Gene Networks, Miyano S, First International Workshop on Computational Methods in Systems Biology, Rovereto, Italy, 24-26 February, 2003.

Towards biopathway modeling and simulation, Miyano, S, The 24th International Conference on Application and Theory of Petri Nets, Eindhoven, The Netherlands, 23-28 July, 2003.

Boundary formation by Notch signaling in Drosophila multicellular systems: experimental observations and gene network modeling by Genomic Object Net, Matsuno H, Murakami R, Yamane R, Yamasaki N, Fujita S, Yoshimori H, Miyano S, The Eighth Pacific Symposium on Biocomputing, Hawaii, USA, 3-7 January, 2003.

Combining microarrays and biological knowledge for estimating gene networks via Bayesian networks, Imoto S, Higuchi T, Goto T, Tashiro K., Kuhara S, Miyano S, The Second International Conference on Computational Systems Bioinformatics, Stanford University, USA, 12-14 August, 2003.

### **Grants**

Miyano S, Research on Information Technology for Gene Network Analysis, Grant-in-Aid for Scientific Research on Priority Areas (C), "Genome Information Science" from MEXT, 1 April 2003-31 March 2004.

Miyano S, Foundations of Computational Knowledge Discovery from Proteome Data, Grant-in-Aid for Scientific Research (B)(1), 1 April 2003 - 31 March 2006.

## **Topics**

### Computational Challenges in Systems Biology.

Systems biology can be explored by development of computational tools and capabilities which enable us to understand complex biological systems. Scientific contributions are strongly anticipated to produce practical benefits such as biomedical applications, solutions for environmental problems, etc. For this purpose, gene networks will play a central role in systems biology and computational challenges to inferring, modeling and simulating biological systems are receiving more attentions.

Advances in measurement technology have enabled genome-wide biological data production. Our challenge in this scope is comprised of two approaches.

The first is "how to create gene network information". For this direction, we have developed three kinds of computational methods for inferring gene networks from gene expression profile data obtained from various perturbations such as gene disruptions, shocks, etc. We developed a method which can analyze the continuous data and automatically detect linear and even nonlinear relationships between genes. We employed nonparametric regression for capturing nonlinear relationships between genes and derive a new criterion called BNRC (Bayesian Network and Nonlinear Regression) for choosing the network in general situations. We also extended this method to dynamic Bayesian network and nonparametric heteroscedastic regression that can cope with time-course microarray data. We have also developed a computational strategy to employ other biological data such as protein-protein interaction data to refine gene networks (Fig. 1). Furthermore, we have developed a gene network analysis tool for extracting subnetworks (Fig. 2).

The second is "how to model and simulate gene networks". Obviously, an important challenge is a creation of a platform with which biological scientists can comfortably model and simulate dynamic causal interactions and processes in the cell such as gene regulations, metabolic pathways, and signal transduction cascades. For this direction, we have developed a software tool Genomic Object Net (GON) (http://www.genomicobject.net/) for biopathway modeling and simulation. We also have developed GONML for describing dynamic biological systems, and simultaneously we have developed a system which converts biopathway models compiled in KEGG and BioCyc to the GONML. Especially, all metabolic pathway models in KEGG are now ready for re-modeling and simulation with GON. With this system, various metabolic pathway information were integrated into a big pathway map so that it can be simulated with GON (Fig. 3).

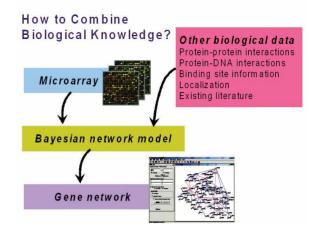


Fig. 1 Employing bilogical information to refine gene network esti-

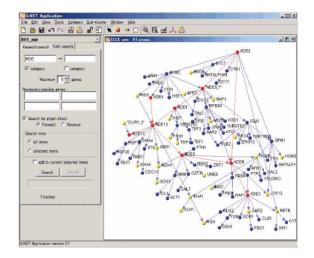


Fig. 2 Gene network analysis tool for network information extraction.

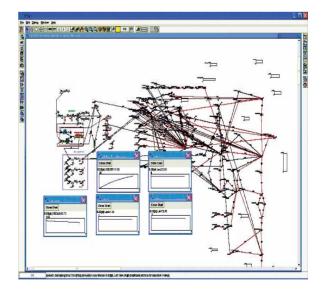


Fig. 3 Modeling and simulation of lac operon gene regulatory network together with metabolic pathways on Genomic Object Net.

# Contributed Chair - Proteome Informatics (SGI Japan) -

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



Vis Assoc Prof MAMITSUKA, Hiroshi (D Sc)



Vis Instr YAMAGUCHI, Atsuko



PD AOKI, Kiyoko F. (Ph D)



PD MAJEUX, Nicolas (Ph D)

### **Scope of Research**

The objective of this laboratory is to establish and develop computationally efficient methods and algorithms utilizing vast amounts of data accumulated from genomics and proteomics to better understand biologically important phenomena. These methods and algorithms form the foundation for analytical systems useful for biology and related fields, such as (bio)chemistry, pharmacology and medical science. Our research themes focus on issues related to proteins, with particular emphasis on protein-protein and protein-ligand interactions.

### **Research Activities (Year 2003)**

### **Presentations**

Predicting Protein-Protein Interactions with Latent Variable Models, Mamitsuka H, Second Asian Joint Workshop on Protein Informatics, Osaka, Japan, 27 February.

Empirical Evaluation of Ensemble Feature Subset Selection Methods for Learning from a High-Dimensional Database in Drug Design, Mamitsuka H, Third IEEE International Symposium on Bioinformatics and Bioengineering, Bethesda, USA, 11 March.

Detecting Experimental Noise in Protein-Protein Interactions with Iterative Sampling and Model-based Clustering, Mamitsuka H, Third IEEE International Symposium on Bioinformatics and Bioengineering, Bethesda, USA, 12 March.

Efficient Unsupervised Mining from Noisy Data Sets, Mamitsuka H, Third SIAM International Conference on Data Mining, San Francisco, USA, 2 May.

Predicting Protein-Protein Interactions with Hierarchical Latent Variable Models, Mamitsuka H, Third Annual Meeting of Protein Science Society of Japan, Sapporo, Japan, 23 June.

Graph Complexity of Chemical Compounds in Biological Pathways, Yamaguchi A, International Workshop on Bioinformatics and Systems Biology, Dresden, Germany, 18 August.

Hierarchical Latent Knowledge Analysis for Cooccurrence Data, Mamitsuka H, Twentieth International Conference on Machine Learning, Washington DC, USA, 23 August. Selective Sampling with a Hierarchical Latent Variable Model, Mamitsuka H, Fifth International Symposium on Intelligent Data Analysis, Berlin, Germany, 30 August.

Efficient Mining from Heterogeneous Data Sets for Predicting Protein-Protein Interactions, Mamitsuka H, Fourteenth International Workshop on Database and Expert Systems, Prague, Czech Republic, 3 September.

Current and Future Perspectives of Proteome Informatics, Mamitsuka H, Japan SGI Ltd. Solution Fair 2003, Tokyo, Japan, 5 November.

Finding the Maximum Common Subgraph of a Partial k-Tree and a Graph with a Polynomially Bounded Number of Spanning Trees, Yamaguchi A, 14th Annual International Symposium on Algorithms and Computation, Kyoto, Japan, 15 December.

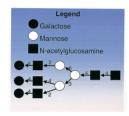
Efficient Tree-Matching Methods for Accurate Carbohydrate Database Queries, Aoki K, Fourteenth International Conference on Genome Informatics, Tokyo, Japan, 16 December.

### Grant

Mamitsuka H, Developing Algorithms for Searching and Finding Small Chemical Compounds Binding to Large Biological Molecules, Grant-in-Aid for Scientific Research on Priority Areas (C), 1 April 2003 - 31 March 2004.

## Algorithms and Statistical Analysis of Structural and Functional Properties of Glycans

Glycans, or carbohydrate chains, are "tree"-like structures consisting of monosaccharides and are vital for the development and function of complex multicellular organisms. However, little progress has been made in this field called glycobiology compared to the tremendous progress made in recent years in DNA and proteomics research. This is largely due to the complexity of the biosynthesis and inherent structure of carbohydrate chains. Thus, we have developed a core of algorithms called KEGG Carbohydrate Matcher (KCaM) for querying glycan chains and performed some preliminary statistical analyses that have been promising. KCaM has been incorporated into the KEGG Glycan database.



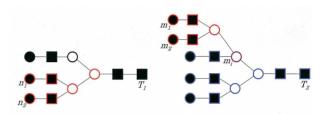
**Figure 1.** KEGG Glycan ID G00281, an N-linked glycoprotein known to be the primary structure of asialo-carbohydrate units.

Figure 1 is an example of a glycan chain. In graph theoretic terms, each node corresponds to a monosaccharide, and each edge corresponds to a linkage. Note that glycan structures start from the right end, where the root node is located, and branch out toward the left. Each such structure is stored in the KEGG Glycan database, but the usefulness of a database cannot be realized unless it can be queried. This is what prompted the development of KCaM, which is based on existing, known methodologies in theoretical computer science and bioinformatics and consists of two variations; a matching algorithm utilizing dynamic programming and which handles gaps, and one that disallows gaps and finds the largest common subtree based on linkage information.

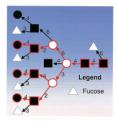
Specifically, KCaM finds the maximum common subtree of two trees,  $T_1$  and  $T_2$ , starting by comparing the leaves of  $T_1$  and  $T_2$  and then moving upward towards the root. This was combined with the Smith-Waterman algorithm, so that each node  $n_1$  from  $T_1$  that forms a match with node  $m_1$  from  $T_2$  stores its match score plus the match information for its children. Every combination of nodes is compared in this way, and the subtree with the largest number of matches, which can be found by following the match information at the root and traversing its children

down to the leaves, is returned as the final result.

For illustration purposes, Figure 2 compares the glycan of Figure 1, which we call  $T_I$ , with a fictional glycan  $T_2$ . In this figure, the nodes that are red and purple indicate a match with the red nodes of  $T_I$ , but the blue and purple nodes are actually a better match since it corresponds with all of the nodes in  $T_I$ . That is, when node  $n_I$  is compared with  $m_I$ , traversing up to node  $m_I$ , only the red nodes match, but in the pass through the algorithm where node  $m_I$  is initially matched with  $n_I$ , we end up matching more nodes by the time the comparisons end at the root. Figure 3 illustrates one of the actual resulting matches with the glycan in Figure 1.



**Figure 2.** In one pass through the KCaM algorithm where when node  $n_I$  is compared with  $m_I$ , traversing up to node  $m_I$ , only the red nodes match. However, in the pass where  $n_I$  is matched with  $m_I$ , we end up matching more nodes by the time the comparisons end at the root.



**Figure 3.** KEGG Glycan ID G05644, with match results with Figure 1 in red. This structure is also an N-linked glycoprotein, published by Yamashita et. al., used in the study of the binding properties of complex-type oligosaccharides on Datura stramonium lectin.

In analyzing the resulting scores from KCaM, the distribution of a random sampling of these scores follows an extreme value distribution, similar to those of sequence similarity scores. We have additionally started incorporating richer information into KCaM in the form of score matrices. Using the scores of matches over the entire KEGG Glycan database, we are developing score matrices taking into account the parent-child relationships in glycan structures. Thus, we can reveal common patterns found in glycans, possibly defining new classes of glycans, and we can statistically estimate the parent-child linkages that frequently appear. Using such tools may assist glycobiologists by providing the clues necessary to glean more detailed information about not only the structure, but also the function of glycans as well.

# **Bioinformatics Center** - Bioinformatics Training Unit -

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



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Vis Assoc Prof KUMA, Keiichi (D Sc)



Vis Instr DAIYASU, Hiromi (D Sc)



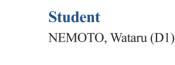
Vis Instr ICHIHARA, Hisako



PD YOKOI, Toshiro (D Agr)



Res HOSOE, Yuko



### 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 2003)

### **Presentations**

Study on the change of constraints associated with the topological change of membrane proteins, Toh H, Ichihara H, Daiyasu H, 3rd Japan Protein Science Society of Japan, 23 June, 2003.

Analysis of sites involved in the functional difference between cryptochrome and photolyase, Daiyasu H, Toh H, 3rd Japan Protein Science Society of Japan, 24 June, 2003

Phylogenetic tree among three domains: horizontal gene transfers and origin of Eukarya, Kuma K, 5th Society of Evolutionary Studies, Japan, 3 August, 2003.

Development of HocDB (Homology-based clustering DataBase), a sequence classification system for database searching, Ishikawa M (Mitsubishi Space Software Co. Ltd.), Sato Y (Mitsubishi Space Software Co. Ltd.), Toh H, 4th Annual meeting of the Chemo-Bioinfomatics Society, 18 September, 2003.

A current wave for the study of protein function, Toh H, Bioinformatics Course of KAST education, 20 October, 2003.

Molecular phylogenetic analysis of pulmonary surfactant-associated protein C and the relatives, Osaka K (Mitsubishi Pharma. Co.), Takei T (Mitsubish Pharma Co.), Toh H, 39th Annual meeting of Japanese Medical Sciety for Biological Interface, 1 November, 2003.

Bioinformatics for prediction of protein function, Toh H, Senri Life Science Sminar, 11 November, 2003.

Evolutionary analysis of membrane-associated proteins, Toh H, Workshop France-Japan on Structural Genomics, 12 November, 2003.

Prediction of protein function and drug design, Toh H, Genomic Drug Design Forum, 17 November, 2003.

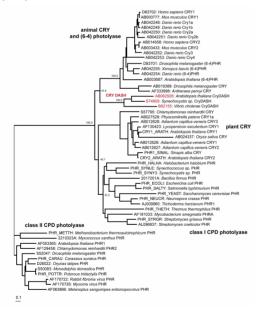
Evolutionary analysis of membrane-associated proteins, Toh H, Ichihara H, Daiyasu H, 10th Congress of the Federation of Asian and Oceanic Biochemists and Molecular Biologists, 10 December, 2003.

The evolutional relationship between genome size and nucleotide composition, Kuma K, Hoshiyama D (Grad.

## Identification of a new cryptochrome class. Structure, function, and evolution.

Cryptochrome flavoproteins, which share sequence homology with light-dependent DNA repair photolyases, function as photoreceptors in plants and circadian clock components in animals. The presence of a new cryptochrome class in bacteria and plants was suggested by a phylogenetic analysis. Coupling studies of sequencing of Arabidopsis cryptochrome gene with the X-ray crystallographic study and biochemical characterization supported the prediction by the phylogenetic study. That is, The crystallographic structure of Synechocystis DASH reveals commonalities with photolyases in DNA binding and redox-dependent function, despite distinct active-site and interaction surface features. Whole genome transcriptional profiling together with experimental confirmation of DNA binding indicated that Synechocystis cryptochrome DASH functions as a transcriptional repressor. The new class of cryptochrome was named DASH.

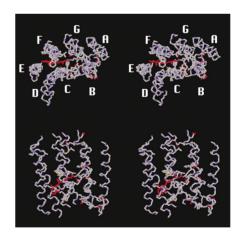
Brudler R, Hitomi K, Daiyasu H, Toh H, Kucho K, Ishiura M, Kanehisa M, Roberts VA, Todo T, Tainer JA, Getzoff ED, *Mol Cell.***11(1)**, 59-67 (2003).



# Archaeal-type rhodopsins in Chlamydomonas: model structure and intracellular localization.

Phototaxis in the unicellular green alga, Chlamydomonas reinhardtii, is mediated by rhodopsin-type photoreceptor(s). Recent expressed sequence tag database from the Kazusa DNA Research Institute has provided the basis for unequivocal identification of two archaeal-type rhodopsins in it. One is located near the eyespot, wherein the photoreceptor(s) has long been thought to be enriched, along with the results of bioinformatic analyses. Secondary structure prediction showed that the second putative transmembrane helices (helix B) of these rhodopsins are rich in glutamate residues, and homology modeling suggested that some additional intra- or intermolecular interactions are necessary for opsin-like folding of the N-terminal ca. 300-aa membrane spanning domains of 712 and 737-aa polypeptides. These results complement physiological and electrophysiological experiments combined with the manipulation of their expression.

Suzuki T, Yamasaki K, Fujita S, Oda K, Iseki M, Yoshida K, Watanabe M, Daiyasu H, Toh H, Asamizu E, Tabata S, Miura K, Fukuzawa H, Nakamura S, Takahashi T, *Biochem Biophys Res Commun*, **301(3)**, 711-717 (2003).



Sch. of Sci., Kyoto Univ.), Katoh K (Grad. Sch. of Sci., Kyoto Univ.), 26th The Molecular Biology Society of Japan, 12 December, 2003.

Molecular phylogenetic analysis of a novel cryptochrome subfamily, DASH, Daiyasu H, Kuma K, Ishikawa T (Rad. Biol. Center., Kyoto Univ.), Todo T(Rad. Biol. Center., Kyoto Univ.), Toh H, 26th The Molecular Biology Society of Japan, 12 December, 2003.

### **Grants**

Toh H, Development of the tools for protein structure comparison, BIRD, 1 April 2003 - 31 March 2004.

Toh H, Domain Prediction in Structural Genomics for Signal Transduction (Inagaki group), Protein 3000, 1 April 2003 - 31 March 2004.

# **Nuclear Science Research Facility**- Particle and Photon Beams -

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



Prof NODA, Akira (D Sc)



Assoc Prof IWASHITA, Yoshihisa (D Sc)



Instr SHIRAI, Toshiyuki



Techn TONGU, Hiromu



PD (NIRS) TAKEUCHI, Takeshi (D Sc)

## Lecturer (pt) Prof TANABE, Tetsumi (D Sc)

Sc) KEK, Japan

### **Students**

NAKAMURA, Shu (D2) YAMAZAKI, Atsushi (D1) TANABE, Mikio (M1) FADIL, Hicham (D2) FUJIMOTO, Shinji (D1) IKEGAMI, Masahiro (D2) MIHARA, Takanori (M2)

### **Visitors**

Dr SYRESIN, Evgeny Dr SHCHAGIN, Alexander V. Prof ROTH, Markus Prof MESHKOV, Igor N. Dr GRIESER, Manfred Dr REISTAD, Dag Dr KAPIN, Valeri Prof SHEVELKO, Viatcheslav P. Prof BULANOV, Sergei V. JINR, Dubna, Russia, 9 January, 29 August - 3 September, 2003 Kharikov Institute of Physics and Technology, Ukraine, 10 February, 2003 Technische Universität Darmstadt, Germany, 17-21 February, 2003 JINR, Dubna, Russia, 7 May, 2003 MPI für Kernphysik, Heidelberg, Germany, 12 -16 May, 2003 The Svedberg Laboratory, Uppsala, Sweden, 16 May, 2003 Moscow Engineering Physics Institute, Russia, 19 September, 2003 P.N. Lebedev Physical Institute, Moscow, Russia, 16 October, 2003 Institute of General Physics, Moscow, Russia, 11 December, 2003

### Scope of Research

Particle and photon beams generated with accelerators and their instrumentations both for fundamental research and practical applications are studied. The following subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Radiation mechanism of photons by electrons in the magnetic field: R&D to realize a compact synchrotron dedicated for cancer therapy; and Irradiation of materials with particle and photon beams.

### Research Activities (Year 2003)

### **Presentations**

Approach to ultra-cold beam at LSR, Kyoto University, Noda A, Joint 28th ICFA Advanced Beam Dynamics & Advanced & Novel Accelerators Workshop on QUANTUM ASPECTS OF BEAM PHYSICS, 11 January, 2003.

Laser-Produced Ion Beam Combined with the RF Accelerator, Noda A, Nakamura S *et al.*, Joint 6th ICFA Advanced & Novel Accelerators and 29th ICFA Advanced Beam Dynamics Workshop on Laser-Beam Interactions, 11 July, 2003.

Ion beam cooling at S-LSR project, Noda A, Shirai T, Fadil H, Ikegami M, Takeuchi T, Noda K, Grieser M *et al.*,

The International Workshop on Beam Cooling, 20 May, 2003.

Hot Ion Beam Electron Cooling Experiments at TSR, Fadil H, Shirai T, Noda A, Grieser M *et al.*, Annual Meeting Phys. Soc. Jpn., 29 March, 2003.

Design of Compact Ion Cooler Ring, LSR for Beam Physics, Shirai T, Ikegami M, Takeuchi T, Tongu H, Noda A *et al.*, Annual Meeting Phys. Soc. Jpn., 29 March, 2003.

Nondestructive Electron Beam Monitor using MCP, Fujimoto S, Shirai T, Iwashita Y, Noda A, Annual Meeting Phys. Soc. Jpn., 29 March, 2003.

Design of Bending Magnet for Ion Storage Ring, LSR, Ikegami M, Shirai T, Takeuchi T, Tongu H, Noda A *et al.*,

# **Topics**

#### Ion Cooler Ring, S-LSR

Particle beams generated by an accelerator behave like rays on the laboratory system but on the center-of-mass system of the beams, the motions of the particles are random and independent between each other. This status corresponds to the gas phase of the matter. The reduction of the relative motion of the particles is one of the most important subjects of the beam physics. It leads to the reduction of the beam size and the increase of the beam density. The ultimate limit of the reduction of the relative motion and the increase of the ion density is a phase transition to a liquid phase and a crystal phase.

Recently the molecular dynamics computer simulations predict the possibility of such phase transitions of the ion beams [1]. The required conditions are a strong beam cooling and a small heating from an accelerator. A laser cooling method is best suited for the first condition. It is applicable for the storage ring, not only for the ion trap [2]. In the second condition, the beam heating comes from the various field errors in the accelerator. The important point is not only decreasing the field error, but also avoiding the resonance between the particle motions and the field errors. From the simulations, the smaller betatron phase advance in an accelerator is considered to be better to avoid the resonane. The predicted upper limit of the phase advance is 127 degree per period [1].

The new ion cooler ring (S-LSR) is under construction at Nuclear Science Research Facility, Institute for Chemical Research [3]. Figure 1 shows the illustration of the ring. Its circumference is 22.557m. It has a laser cooler for Mg<sup>+</sup> with the laser wavelength of 280 nm. The ring satisfies the phase advance less than 127 degrees and its minimum phase advance is 87 degrees [4]. High precision of the magnet fabrications, stable power supplies and good alignments are in pursuit for the small field errors. Figure 2 shows the photograph of the bending magnet and the quadrupole magnet. The deviation of the magnetic field strength among



Figure 1 Schemmatic view of new ion cooler ring, S-LSR



**Figure 2** Top view of a bending magnet and a quadrupole magnet for S-LSR.

6 bending magnets is less than  $10^{-4}$ . The filed stability is less than  $10^{-5}$  [5].

S-LSR has also an electron cooler, which can cool various ion species and suited for the reserches, such as a short bunch beam formation, which can provide a new tool of the pulse radiolysis by ion beams [6]. S-LSR has a fast kicker to extract the short bunch beam.

- 1. Wei, J et al., Phys. Rev. Lett. 73 (1994) 3089
- 2. Hangst, J.S. et al., Phys. Rev. Lett. 67 (1991) 1238
- 3. Noda, A et al., Proc. of the 2002 EPAC, France, (2002) 2750
- 4. Shirai, T et al., Proc. of the 2002 EPAC, France, (2002) 623
- 5. Ikegami, M et al., Proc. of SAST03 (2003) 184
- 6. Noda, K et al., Proc. of the 2002 EPAC, France, (2002) 1380

Annual Meeting Phys. Soc. Jpn., 29 March, 2003.

Development of Quadrupole Magnet for Compact Ion Storage Ring, Takeuchi T, Shirai T, Ikegami M, Tongu H, Noda A *et al.*, Annual Meeting Phys. Soc. Jpn., 31 March, 2003.

Final Focus Lens using Super Strong Permanet Magnet Quadrupole in Linear Collider, Mihara T, Iwashita Y, Kumada M, Aoki M, The 14th Symposium on Accelerator Science and Technology, 11 November, 2003.

Final Focus Lens using Permanent Magnet in Linear Collider, Iwashita Y, Kumada M, Aoki M *et al.*, Annual Meeting Phys. Soc. Jpn., 31 March, 2003.

Velocity Compliant Bunching Scheme with Amplitude

Modulation, Iwashita Y, 5th International Workshop on Neutrino Factories, 6 June, 2003.

#### **Grants**

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

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

Iwashita Y, Basic Research on the Table-top Neutron Source, REIMEI Research Resources of JAERI, April 2003 - March 2004.

# **Nuclear Science Research Facility**- Beams and Fundamental Reaction -

(1) http://www.scl.kyoto-u.ac.jp/~sakabe/index.html (2) http://carrack.kuicr.kyoto-u.ac.jp/

#### (1) Laser-matter interaction science



Prof SAKABE, Shuji (D Eng)



Instr HASHIDA, Masaki (D Eng)

#### (2) Astroparticle and atomic physics



Prof MATSUKI, Seishi (D Sc)

# Researcher TADA, Masaru (D Sc)

#### **Students** KOMINATO, Kentaro (D3) SHIBATA, Masahiro (D3)

#### Scope of Research

#### (1) Laser-matter interaction science

Physics of matter in strong optical field created by powerful lasers is studied. With ultra-intense intense femtosecond laser, ionization and Coulomb explosion of large molecules and clusters, and high energy radiation (x-ray, electrons, ions) generation in plasmas are of our interest to open a new field of laser nuclear science.

#### (2) Astroparticle and atomic physics

Dark matter particles in the Universe are studied with quantum electronic methods: Search for a dark-matter candidate, axion, in the Universe with Rydberg atoms, and related characteristics of Rydberg atoms in external fields.

### Research Activities (Year 2003)

#### **Presentations**

#### (1) Laser-matter interaction science

Anisotropic Coulomb explosion of Ar cluster induced by an intense femtosecond-laser pulse, S. Shimizu, M. Hirokane, M. Hashida, S. Okihara, Y. Izawa, S. Sakabe, International Symposium on Ultrafast Intense Laser Science 2: Propagation and Interaction, Quebec, Canada, 27 -29 September.

Molecular deformation of benzene and fluorinated benzene in explosion processes induced by intense femtosecond-laser pulses, S. Shimizu, V. Zhakovskii, M. Murakami, T. Yatsuhashi, K. Nishihara, S. Sakabe, Y. Izawa, N. Nakashima, International Symposium on Ultrafast Intense Laser Science 2: Propagation and Interaction, Quebec, Canada, 27 - 29 September.

Femtosecond laser ablation of metals: characterization

of new processing phenomenon and formation of nanostructures, M. Hashida, S. Nagashima, M. Fujita, M. Tsukamoto, M. Katto, and Y. Izawa, 9th Symposium on Microjoining and Assembly Technology in Electronics (Mate), Yokohama, Japan, 6 - 7 February.

Periodic structure of metals with femtosecond laser ablation, M. Hashida, M. Fujita, M. Tsukamoto, Y. Izawa, and A. F. Semerok, 2003 Conference on Lasers and Electro-Optics Europe (CLEO/Europe), Munich, Germany, 23 - 27 June.

#### (2) Astroparticle and atomic physics

Zerofield crossings in the pulsed field ionization under a rotating electric field, Shibata M, Kishimoto Y, Tada M, Yamada S, Kominato K, Haseyama T, Funahashi H, Yamamoto K, and Matsuki S, Autumn Meeting, Phys. Soc. Jpn.,

#### (1) Laser-matter interaction science

# Generation of high energy protons from hydrogen clusters Coulomb-exploded by intense femtosecond laser pulses

Energy distributions of protons emitted from hydrogen clusters Coulomb-exploded by an intense femtosecond laser have been experimentally obtained. 10,000-hydrogen clusters were exploded to emit 8.1 keV protons under laser irradiation of intensity  $6\times10^{16}$  W/cm². The energy distributions are interpreted well by a spherical uniform cluster analytical model for the first time. The maximum energy of emitted protons can be characterized by cluster size and laser intensity. The laser intensity scale for the maximum proton energy, given by a spherical cluster Coulomb explosion model, is in fairly good agreement with the experimental results obtained at the laser intensity of  $10^{16}$ - $10^{17}$  W/cm² and also when extrapolated to the results of three dimensional particle simulations at  $10^{20}$ - $10^{21}$  W/cm².

#### Ion generation in a low-density plastic foam by interaction with intense femtosecond laser pulses

Energetic proton generation in low-density plastic (C<sub>5</sub>H<sub>10</sub>) foam by intense femtosecond laser pulse irradiation has been studied experimentally and numerically for the first time. Plastic foam was successful produced by a solgel method, achieving an average density of 10 mg/cm<sup>3</sup>. The foam target was irradiated by 100-fs pulses of a laser intensity 1×10<sup>18</sup> W/cm<sup>2</sup>. A plateau structure extending up to 200 keV was observed in the energy distribution of protons generated from the foam target, with the plateau shape well explained by Coulomb explosion of lamella in the foam. The laser-foam interaction and ion generation were studied qualitatively by two-dimensional Particle-in-Cell (PIC) simulations, which indicated that energetic protons are mainly generated by the Coulomb explosion. From the results, the efficiency of energetic ion generation in a lowdensity foam target by Coulomb explosion is expected to be higher than in a gas-cluster target.

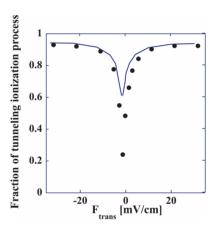
#### Okayama, 22 September.

Autoionization process in the highly excited Rydberg atoms of Rb, Yamada S, Kishimoto Y, Tada M, Shibata M, Kominato K, Haseyama T, Funahashi H, Yamamoto K, and Matsuki S, Autumn Meeting, Phys. Soc. Jpn., Okayama, 22 September.

#### (2) Astroparticle and atomic physics

#### Zero-field crossing in the pulsed-field ionization processes under a rotating electric field

Rydberg atoms have been widely utilized for fundamental physics researches. In order to extend further the applicability of the Rydberg atoms in higher excited states[1], we developed new stringent schemes to selectively ionize highly excited Rydberg atoms by manipulating the ionization path in a Stark map[2]: In one of these schemes, zerofiled crossing during the course of the pulsed field ionization under a rotating electric field plays a key role for improving the selectivity. Underlying physics in these issues is the rotation of the state angular momentum due to the rotating electric field: Specifically with this rotation effect, the tunneling ionization process increases profoundly compared to the autoionization-like process. In Fig.1 shown is the fraction of the tunneling ionization in the n=112 manifold states of 85Rb as a function of the applied transverse electric filed. Quantum theoretical predictions (solid line) reproduce fairly well the experimental results.



**Fig.1** Fraction of the tunneling field ionization process as a function of the applied transverse electric field in the n=112 manifold states of Rb. The fraction increases abruptly with increasing transverse field, indicating a profound effect of the rotating electric field on the substate redistribution of the total angular momentum.

1. T. Haseyama et al., Phys. Lett. A317 (2003) 450.

2. M. Tada, et al., Phys. Lett. A303 (2002) 285;Y. Kishimoto et al., Phys. Lett. A303 (2002) 279.

#### **Grants**

Sakabe S, Fundamental Research on  $\gamma$ -ray laser with intense femtosecond lasers, Grant-in-Aid for Scientific Research (B)(2), 1 April 2003 - 31 March 2005.

Sakabe S, Research on Coulomb Explosion Dynamics of Cluster Molecules with intense lasers, Grant-in-Aid for Scientific Research Priority Areas (C), 1 April 2003 - 31 March 2004.

# Laboratories of visiting professors

#### **Solid State Chemistry**



Vis Prof INOUE, Jun-ichiro (D Eng)

Professor, Graduate School of Engineering, Nagoya University (Furo-cho, Chikusa-ku, Nagoya 464-8603)

#### Lectures at ICR

Magnetoresistance in Exchange-Spring Multilayers with Twisted Spin Structures (Theories)

Recent Topics on Spintronics

Magnetism - From Fundamentals to Spintronics I

Magnetism - From Fundamentals to Spintronics II

Magnetism - From Fundamentals to Spintronics III



Vis Assoc Prof YAMANAKA, Akio (D Sc)

Professor, Chitose Institute of Science and Technology (CIST) [Promoted on 1 April 2003] (758-65, Bibi, Chitose, Hokkaido 066-8655)

# **Lecture at** *ICR* Raman Scattering Study of Solids

#### **Fundamental Material Properties**



Vis Prof YABUKI, Kazuyuki (D Eng)

Associate Director, General Manager, Tsuruga Center, Toyobo Co., Ltd. (10-24, Toyo-cho, Tsuruga, Fukui 914-8550)

#### Lectures at ICR

Properties and Applications of High-Performance Fibers

- (1) Relation between polymer chain rigidity and physical properties of fibers
- (2) Structure and properties of PBO fiber
- (3) Ultra high molecular weight PE fiber
- (4) Fatigue mechanism of fibers
- (5) Development of applications for super fibers



Vis Assoc Prof **SATO, Takaya** (D Eng)

Chief Scientist, R&D Center, Nisshinbo Industries Inc. (1-2-3, Ohnodai, Midori-ku, Chiba 267-0056)

#### Lectures at ICR

Electrochemical Properties of Quaternary Ammonium Ionic Liquid for Electrolyte Applications

High Performance Electric Double Layer Capacitor Using Novel Ionic Liquid The Application of Ionic Conductive Cellulose Derivatives for Rechargeable Lithium Polymer Battery

#### **Synthetic Organic Chemistry**



Vis Prof YAMAMOTO, Yohsuke (D Sc)

Professor, Faculty of Science, Hiroshima University (1-3-1 Kagamiyama, Higashi-Hiroshima, 739-8526)

#### Lecture at ICR

Syntheses and Structures of Five-coordinated Carbon and Boron Compounds



Vis Assoc Prof SUGIO, Shigetoshi (D Pharm Sc)

Senior Research Associate, Science & Technology Office, Yokohama Center, Mitsubishi Chemical Corporation (1000, Kamoshida, Aoba-ku, Yokohama 227-8502)

#### Lectures at ICR

Genomic Drug Discovery: A Paradigm for Drug Discovery in Post-Genome Era Recent Advances in Structural Biology

#### **International Research Center for Elements Science**



Vis Prof TATSUMI, Kazuyuki (D Eng)

Professor, Research Center for Materials Science, Nagoya University (Furo-cho, Chikusa-ku, Nagoya 464-8602)

#### Lecture at ICR

Transition Metal Sulfides -Synthetic Models of the Nitrogenase Active Sites (10 Jan. 2004)



Vis Assoc Prof YANO, Yoshihiko (D Eng)

Chief Scientist, Research & Development Center, TDK Corporation (2-15-7, Higashi-Ohwada, Ichikawa, Chiba 272-0026)

Lecture at *ICR*Inorganic EL Device

# **International Research Center for Elements Science (Foreign Guest Laboratory)**



Vis Prof LIU, Yunqi (D Eng)

Professor, Institute of Chemistry, Chinese Academy of Sciences [Term of visit: 5 January-4 April 2004] (No. 2, 1st North Street, Zhongguancun Beijing 100080, China)

#### Lectures at ICR

Electronic Devices Based on Multiwalled Carbon Nanotubes (10 Jan. 2004) Organic/polymeric Light-emitting Diodes (22 Jan. 2004) Phthalocyanines: Synthesis, Characterization and Their Application in Electronic Devices (22 Jan. 2004)

# Personal

#### Retirement

Professor UEDA, Kunihiro

(Molecular Clinical Chemistry,
Bioorganic Chemistry)



On the 31st of March 2004, Dr. Kunihiro Ueda retired from Kyoto University after 34 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Ueda was born in Kyoto on 25th of May, 1940. He graduated from Kyoto University Faculty of Medicine in 1965 and finished an internship at Kyoto University Hospital in 1966. He studied medical chemistry at the Graduate School of Medicine, Kyoto University, under the supervision of Professor O. Hayaishi, and was granted a doctoral degree in 1973. In 1971, he was appointed as an instructor of the Institute for Chemical Research, Kyoto University. On leave from Kyoto University from 1974 to 1976, he studied molecular biology under Professor A. Kornberg at Stanford University, USA. In 1981, he was promoted to a Lecturer of Medical Chemistry and, in 1985, an Associate Professor of Clinical Science and Laboratory Medicine, Kyoto University. In 1994, he was appointed as a full Professor of the Institute for Chemical Research, Kyoto University, and directed the Laboratory of Molecular Clinical Chemistry. He gave lectures at the Graduate School of Medicine and supervised the dissertation works of graduate students.

During his academic carrier, Dr. Ueda made a number of notable findings regarding the regulatory mechanisms of life. In particular, the discovery of "the third nucleic acid", i.e. poly(ADP-ribose), with Dr. Y. Nishizuka in 1966 opened a new era of protein modification by coenzyme, NAD<sup>+</sup>, and led him to a life-long enthusiasm for research of this novel polymer. His years' effort resulted in the discovery and characterization of three key enzymes, one synthetic and two degradative, in poly(ADP-ribose) metabolism, isolation of poly(ADP-ribosyl) histones from animal tissues, immunohistochemical demonstration of poly(ADP-ribose) in human cells, finding of roles of poly(ADP-ribose) in DNA repair, carcinogenesis and apoptosis, development of specific inhibitors of the synthetase, and discovery of the inhibitors' protective effects

against ischemic or oxidative lesions in the brain and heart. All these achievements formed landmarks in the history of poly(ADP-ribose) research and made Dr. Ueda one of the leaders in this research field in the world.

After moving to a clinical laboratory, he also undertook investigation of molecular etiology of Alzheimer's disease and improvement of gene diagnostic techniques. His early finding of an age-related change in expression of  $A\beta$  amyloid precursors among patients was a pioneering work in understanding the pathogenesis of Alzheimer's. He later disclosed a possible link between overactivation of poly(ADP-ribose) synthesis and neuronal degeneration in this disease. His efforts in developing methods for clinical gene testing resulted in commercialized products, Ampdirect<sup>TM</sup> for polymerase chain reaction and a transcription-reverse transcription-concerted reaction device.

For these distinguished contributions to science and biotechnology, he was awarded the Young Researcher Promotion Prize from the Japanese Biochemical Society, the Prize of the Japan Society of Vitaminology and Nutrition, and the Shibata Susumu Medal from the Clinical Pathology Promotion Foundation.

He served in the three Ministries' Joint Committee for Ethics Guidelines for Human Genome/Gene Analysis Research. He chaired the Committee for Regulation of Human Genome/Gene Analysis Research in Kyoto University. He served as members of Directors of many academic societies in Japan and has kept the presidency in the Society for Gene Diagnosis and Therapy since 2001. Internationally, he organized the First Japan-Italy Bilateral Seminar on ADP-riboses and Nitric Oxide (1997, Kyoto) and the Second IFCC-Roche Conference on Human Genomics (2000, Kyoto). He is an International Editor of the *Annals of Clinical Biochemistry* and the *Journal of Enzyme Inhibition and Medicinal Chemistry*.

His contribution to Kyoto University through both academic and administrative activities is gratefully acknowledged.

#### Retirement

Professor MATSUKI, Seishi
(Beams and Fundamental Reaction,

Nuclear Science Research Facility)



On the 31st of March, 2004, Dr. Seishi Matsuki retired from Kyoto University after 27 years of service to the University. Dr. Seishi Matsuki was born in Kami-shibetsu, Hokkaido on March 19, 1941. After graduated from the Department of Physics, Faculty of Science, Kyoto University in 1963, he continued his study on nuclear physics in Graduate School of Physics, Kyoto University under the supervision of the late Professor Takuji Yanabu. He finished the Doctor Course of Physics, and was granted a doctoral degree of Science, Kyoto University in 1968.

After continued physics research in the group of Professor Yanabu as a Post Doctoral researcher of Japan Society for the Promotion of Science, he was appointed to an instructor of the Nuclear Engineering Department, Kyushu University in 1969. He moved to the Department of Physics, Nara Women's University as an Associate Professor of physics in 1972 and then belonged to Nuclear Science Research Facility, Institute for Chemical Research, Kyoto University as an Associate Professor in 1977. He was promoted to a full Professor of Institute for Chemical Research, Kyoto University in 2003. He stayed at the Heavy-ion Physics Laboratory (GSI) in Darmstadt, Germany for one year in 1978-1979 as a Humboldt research fellow.

During his academic carrier, Dr. Matsuki has been involved in the study of nuclear, particle and related astro-particle physics. He studied nuclear reactions and nuclear structure during the early period in Kyoto and in Kyushu. One of his remarkable achievements during this period is the systematic observation of the isobaric analog resonances in the  $(p,n\gamma)$  reactions. He clarified the lowlying level structure of Nb nuclei with these resonances. He also started to be involved in the particle and related astro-particle physics in Nara and Kyoto period. After he belonged to the Institute for Chemical Research, he started

to apply lasers and quantum electronic techniques to the study of nuclear and particle physics. One of the novel results he obtained along this line is that he achieved the nuclear polarization of more than 30% for In nuclei in InP semiconductors with a laser-assisted Overhauser process. This achievement opened an efficient way to polarize unstable nuclei.

For the recent years he devoted himself to the investigation of dark matters in the Universe with a funding support of a Grant-in-Aid for Specially Promoted Research by the Ministry of Education, Culture, Sports, Science and Technology, Japan. Specifically he developed a quite sensitive microwave single-photon detector with high Rydberg atoms to search for axions, one of the most elegant candidate particles for the dark matter. Related to this research, he also obtained many invaluable findings on the structure of Rydberg atoms and their applications to fundamental researches.

He gave lectures on nuclear and particle physics since 1978 at the graduate school of physics, Kyoto University, and was charged with supervising dissertation works of a number of graduate students. He was a visiting lecturer at many Universities such as Osaka and Kyushu University. He served as a member of the program committee of the Physical Society of Japan. He also served as a member of the international organizing committee of several international conferences on dark matter and nuclear physics.

His contribution to the University through his scientific, educational and administrative activities is hereby gratefully acknowledged.

# **Awards**

# OKITOH, Norihiro



**Humboldt Research Award** (Alexander von Humboldt Foundation)

"Systematic Studies on Homo- and Heteronuclear Doubly Bonded Compounds between Heavier Group 15 Elements"

Awarded for the accomplishments in his research on organoelement chemistry, particularly for (1) the creation of novel homo- and heteronuclear doubly bonded systems between heavier group 15 elements as stable compounds utilizing kinetic stabilization, e. g., the first synthesis of stable dibismuthene (RBi=BiR; the heaviest double-bond compound) and phosphabismuthene (RP=BiR; a novel heteronuclear double-bond compound), and (2) the systematic elucidation of the structures and properties of these novel doubly bonded systems.

7 November 2003

Originally founded in 1860 in memory of eminent scientist Alexander von Humboldt, the Alexander von Humboldt Foundation set up the Research Award, which is, after two interruptions by World Wars, now conferred to up to 100 most prominent researchers world-wide every year in all academic fields covering from natural science to the humanities.



The Chemical Society of Japan Award for Creative Work (The Chemical Society of Japan)

"Synthesis of Aromatic Species Containing a Heavier Group 14 Element by Taking Advantage of Kinetic Stabilization"

20 March 2003

KURATA, Hiroki



The Japanese Society of Microscopy Award

"Development of Electron Energy-loss Spectroscopy and Its Application to Local State Analysis of Materials" The Japanese Society of Microscopy

8 June 2003

SOHRIN, Yoshiki



18th Oceanochemistry Award

"Analysis and Dynamics of Trace Metals in the Ocean" Research Institute of Oceanochemistry

28 April 2003

#### TAKAHASHI, Masahide



# Japan-Australasian Ceramic Society Joint Ceramic Award

"Study on the Optical Functional Glasses Doped with Active Centers"

The Ceramic Society of Japan and Australasian Ceramic Society

30 May 2003

#### TSUJII, Yoshinobu



#### **SPSJ Willey Award**

"Synthesis and Properties of Newly Developed Polymer Brushes"

The Society of Polymer Science, Japan

25 September 2003

#### NISHINAGA, Tohru



# Konica Minolta Technology Center Award in Synthetic Organic Chemistry, Japan

"Development of Molecular Wire Insulated by Rigid Carbon-Frameworks and Evaluation of Redox-Based Switching Properties"

The Society of Synthetic Organic Chemistry, Japan

28 November 2003

#### MURATA, Yasujiro



#### The ICR Award for Young Scientists

"Synthesis of Open-Cage Fullerene Derivatives and 100% Encapsulation of a Hydrogen Molecule" ICR

5 December 2003

#### TAKEDA, Nobuhiro



#### Progress Award in Silicon Chemistry, Japan

"Stabilization of Low-coordinated Group 14 Element Compounds by Taking Advantage of Steric Protection"

The Society of Silicon Chemistry, Japan

18 October 2003

#### OHASHI, Yohei



#### The ICR Award for Young Scientists

"Functional Analysis of the *Arabidopsis GLABRA2* Gene That Contributes Root-hair Development through the Modulation of Phospholipid Signaling"

**ICR** 

5 December 2003

#### TAMAO, Kohei



#### The 14th Mukai Prize

"Discovery of Cross-Coupling Reaction and Its Application"

Tokyo Ohka Foundation for Promotion of Science and Technology

5 June 2003

#### YAMANISHI, Yoshihiro



#### The ICR Award for Students

"Extraction of Correlated Gene Clusters from Multiple Genomic Data by Generalized Kernel Canonical Correlation Analysis"

**ICR** 

5 December 2003

#### TAKANO, Mikio



# 2002 JSPM Award for Distinguished Achievements in Research

"Discovery of Novel 3d-Transition Metal Oxide: High-Pressure Synthesis"

The Japan Society of Powder and Powder Metallurgy

21 May 2003

#### ISHIWATA, Shintaro



#### The ICR Award for Students

"High Pressure Synthesis and Crystal Structure of Perovskite BiNiO<sub>3</sub>, and Suppression of A-site Charge Disproportionation by La-substitution"

**ICR** 

5 December 2003

# **Poster Awards**

#### KADOYA, Hidenori



#### **Award for the Best Presentation**

The 30th Annual Meeting of the Society of Rheology, Japan

"Electric Birefringence of Amorphous Polymers" The Society of Rheology, Japan

15 May 2003

MIURA, Masaya



#### **Best Poster Award**

9th Summer Meeting on Functional Host-Guest Chemistry

"Effective Synthesis of Chiral Oligo-Naphthalene Derivatives"

Functional Host-Guest Chemistry, Japan

21 August 2003

SHINOHARA, Akihiro



#### **Symposium Poster Award**

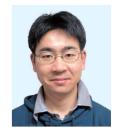
8th Symposium of the Society of Silicon Chemistry, Japan

"Reactivity of Kinetically Stabilized Silaaromatic Compounds"

The Society of Silicon Chemistry, Japan

17 October 2003

KATO, Masahiro



#### **Poster Award**

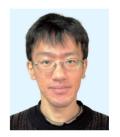
1st International Symposium on Biomolecular Chemistry (ISBC2003)

"Glycosylamidines as Potent and Selective Glycosidase Inhibitors"

Forum on Biomolecular Chemistry (FBC), The Chemical Society of Japan

5 December 2003

SAITO, Shigeki



#### **Poster Award**

The 38th Annual Meeting of The Japanese Society for Chemical Regulation of Plants

"Characterization of Cytochromes P450 involved in ABA Catabolism"

The Japanese Society for Chemical Regulation of Plants

30 October 2003

KAWANO, Shin



#### **Best Poster Award JSPS**

ESF-JSPS Frontier Science Meeting for Young Researchers: Functional Genomics - from the bench to bioinformatics

"Glycoinformatics: Prediction of Glycan Structures Based on Enzymatic Knowledge of Glycosyltransferase Reactions"

ESF (The European Science Foundation) and JSPS (Japan Society for the Promotion of Science)

29 October 2003

# **Obituary**

**Professor Emeritus** 

Dr. SHIGEMATSU, Tsunenobu (1916-2003)



Dr. Tsunenobu Shigematsu, Professor Emeritus of Kyoto University passed away on November 18, 2003 in Kyoto.

Dr. Shigematsu was born on December 28, 1916 in Ehime. He graduated the Department of Chemistry, Faculty of Science, Kyoto Imperial University in 1940. During the war, he was appointed to a lieutenant commander of engineering. After the war, he was appointed to a junior assistant of the Faculty of Science, Kyoto Imperial University in 1947. He was promoted to an instructor of the Faculty of Science, Kyoto University in 1949, moved to the Faculty of Engineering and promoted to a lecturer in 1950. He got a Ph. D. (Doctor of Science) from Kyoto University in this year. He was promoted to an associate professor, the Faculty of Science in 1952. He was promoted to a full professor of the Institute for Chemical Research in 1957 to direct the Laboratory of Radiochemistry, which is presently the Laboratory of Hydrospheric Environment Analysis, Division of Interface Science III. He was appointed to the 16th director of the Institute for Chemical Research and a member of the University Council, Kyoto University from 1976 to 1978, and the director of the Radioisotope Research Center, Kyoto University from 1979-1980. He retired from Kyoto University in 1980, honored with the title of Professor Emeritus of Kyoto University. After the retirement, he served as a professor of the College of Liberal Arts, Kinki University from 1980 to 1991 and appointed to the president of Kinki University Toyooka Women's Junior College from 1985 to 1990.

Dr. Shigematsu produced a lot of brilliant achievements in analytical chemistry, marine chemistry, and radiochemistry, contributing largely to the development of these research fields. His major contributions are as following: (1) Radiochemistry. He determined radio isotopes in the ashes of Bikini nuclear testing. He studied radioactivation analysis and treatment of radioactive waste water. (2) Chemical studies of the ocean. Research on marine chemistry in Japan has been started by Dr. Masayoshi Ishibashi, Professor Emeritus of Kyoto University in 1935. Dr. Shigematsu was the most important successor of the research. He determined many dissolved elements in seawater and discovered the regularities of the amounts of elements in seawater. (3) Spectrochemical Analysis. He developed absorption, fluorescence and atomic absorption spectrometry for trace elements, applying to analysis of seawater and natural water. (4) Solvent extraction. He analyzed the extraction reaction and equilibrium. He developed new ligands for extraction of metal chelates. (5) Coprecipitation. He analyzed coprecipitation as the distribution equilibrium of trace metals between solid and liquid phases.

Dr. Shigematsu was truly a gentle and honest person. He educated many students and younger people. He served as the vice president of the Japan Society for Analytical Chemistry from 1973 to 1974 and the director of its Kinki Branch from 1973 to 1975. For his great academic and educational contributions, Dr. Shigematsu was honored with the Award of the Japan Society for Analytical Chemistry in 1965 and the Second Class of the Order of the Sacred Treasure in 1991.

# **Obituary**

Professor Emeritus

Dr. SHIMIZU, Sakae (1915-2003)



Professor Dr. Sakae Shimizu, Professor Emeritus of Kyoto University passed away on December 13, 2003 in Osaka.

Dr. Shimizu was born on July 18, 1915 in Tokyo. He entered the Department of Physics, Faculty of Science, Kyoto Imperial University in 1935 and was moved up to the Graduate School of Science, Kyoto Imperial University in 1940. After graduation, he appointed to a Lecturer in the Department of Physics, Kyoto Imperial University in 1943 and to an Associate Professor in the same Department in 1946. He got a Ph.D. (Doctor of Science) from Kyoto Imperial University in 1950 and was promoted to a full Professor of the Institute for Chemical Research, Kyoto University in 1952 to direct the Laboratory of Nuclear Radiation (presently, the Laboratory of Atomic and Molecular Physics, Division of States and Structures). From 1957 to 1959, he did his best to promote the Kyoto University Research Reactor and to establish Radioisotope Research Committee of Kyoto University. He also made a main contribution to complete Radioisotope Research Laboratory constructed on the north campus in 1961, which was reorganized and renamed the Radioisotope Research Center in 1971. From 1960 to 1979, he served as the first Director of this Center to promote further researches and educations utilizing radioisotopes in Kyoto University. In this period, he was the chairman of the Radioisotope Research Committee and the Committee for Preparation of Nuclear Research Facilities. He retired from Kyoto University in 1979, honored with the title of Professor Emeritus of Kyoto University.

Dr. Shimizu's research field extended over the wide region concerning with pure nuclear physics as well as its applications to many fields. In the period from 1943 to 1945 of the World War II, he devoted himself to experimental study of photonuclear reaction, construction of the 12" cyclotron and separation of <sup>235</sup>U by the ultra-centrifugal method. In 9-16 August 1945 just before the end of the War, as a member of the first party of Kyoto University and a leader of the second party, he exerted

himself for the field survey of Hiroshima Atomic Bombing (6 August 1945), which contributed to disclose very rabidly the nature of the Bombing. One of his works after the War was the reconstruction of the Kyoto cyclotron completed in 1955. In 1954, with the group composing of nuclear physicists, analytical chemists, medical research workers in Kyoto University, he performed extensive studies on so-called "Bikini Ashes"-radioactive fallout collected aboard of Japanese fishing boat, Lucky Dragon No. 5. He successively informed all over the world of the nature of the terrible explosion, that is the hydrogen bomb newly developed, through the full report rapidly published from the Institute for Chemical Research.

From 1961 till his retirement, his main interest was concentrated to the boundary region between nuclear and atomic physics. Main subjects were 1) External Effects in the Radioactive Constant, 2) Positron Annihilation with K-shell Electrons and 3) K-shell Internal Ionization Accompanying Nuclear Decays. He and his many followers performed a lot of experimental studies on those subjects at his Radioisotope Research Laboratory on the north campus.

As a Member of Board of Education of Kyoto City from 1979 to 1994 and also as the Director of Kyoto Municipal Science Center for Youth from 1970 to 1979, Dr. Shimizu largely contributed to promote the education of science for young generation in Kyoto City. He was one of representative directors of the Japan Radioisotope Association from 1962 to 2000 and, as the Vice President of the Association (from 1990 to 2000), he did his best to extend the use of radioisotopes for scientific researches and various medical purposes in Japan. He was an Honorary Member of Hungarian Academy of Science since 1995, which was presented for his continuous effort to develop the science interchange between Japan and Hungary. For these great academic and educational contributions, Dr. Shimizu was awarded the Third Class of the Order of Rising Sun in November, 1988.

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#### INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

Key Center for Polymer Colloids, School of Chemistry, University of Sydney

[Austria]

Institute of Theoretical Physics, Graz University

[Belgium]

Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven

Laboratory of Nuclear Chemistry, Université Catholique de Louvain

Optique Nonlinéaire Théorique, Université Libre de Bruxelles

[Canada]

Department of Chemical Engineering, McMaster University

[France]

Centre de Geostatistique, Ecole des Mines de Paris

[Germany]

Bioinformatics & Computational Biology, European Molecular Biology Laboratory (Heidelberg)

Department of Physics, Justus Liebig University

Max Planck Institute for Metals Research

Max Planck Institute for Nuclear Physics

[Italy]

Centro di studio per gli Acidi Nucleici, Universita di Roma La Sapienza

Istituto Nazionale di Ricerca per gli Alimenti e la Nutrizione

Laboratori Nazionali di Legnaro, Istituto Nazionale di Fisica Nucleare

[Poland]

Laboratory of Toxicology and Risk Assessment, Institute of Coal Chemistry, Polish Academy of Sciences

[P. R. China]

Department of Chemistry, Lanzhou University

Department of Chemistry, University of Science and Technology of China

State Key Laboratory of Inorganic Synthesis & Preparative Chemistry, Jilin University

[Russia]

Dzhelepov Laboratory of Nuclear Problems, The Joint Institute for Nuclear Research

Plasma Physics Department, General Physics Institute of the Russian Academy Sciences

The Budker Institute of Nuclear Physics

[Sweden]

Institute of Chemistry, Uppsala University

[Switzerland]

Institute of Crystallography, University of Lausanne

Laboratorium für Chemische und Mineralogische Kristallographie der Universität Bern

[Thailand]

Department of Chemistry, Faculty of Science, Mahidol University

[UK]

Centre for Analytical Sciences, Department of Chemistry, University of Sheffield

Department of Chemistry, University of Warwick

Department of Materials, The University of Oxford

[USA]

Center for Environmental and Occupational Risk Analysis and Management, College of Public Health, University of South Florida

Center for X-ray Optics, Lawrence Berkeley National Laboratory

Department of Biology, Colorado State University

Department of Chemistry and Biochemistry, University of California

Department of Chemistry and Biochemistry, University of Colorado

Department of Chemistry, The Scripps Research Institute

Department of Chemistry, University of Georgia

Department of Chemistry, University of Miami

Department of Neurosciences, School of Medicine, University of California San Diego

Department of Molecular Biology and Skaggs Institute for Chemical Biology, The Scripps Research Institute

Department of Physics, Applied Physics, and Stanford Synchrotron Radiation Laboratory, Stanford University

Department of Physics, University of California

Department of Physics, University of Florida

Lawrence Livermore National Laboratory

Molecular and Experimental Medicine MEM275, The Scripps Research Institute

National Radio Astronomical Observatory

National Heart, Lung, and Blood Institute, National Institutes of Health

Polymer Division, National Institute of Standards and Technology

#### THESES

ASAKA, Takao

D Sc, Kyoto University

"Method for Stabilizing Beam Intensity and Energy in the

Spring-8 Linac"

Supervisor: Prof NODA, Akira

25 September 2003

ISHIWATA, Shintaro

D Sc, Kyoto University

"Synthesis and Crystal Growth under High Pressure for

Perovskite Oxides with Charge Disproportionation"

Supervisor: Prof TAKANO, Mikio

24 May 2003

KONDO, Yuki

D Eng, Kyoto University

"Studies on Optical Nonlinearities of Oxide Glasses by Using

Short-Pulse Lasers"

Supervisor: Prof YOKO, Toshinobu

23 March 2003

MIYAZAKI, Tsukasa

D Eng, Kyoto University

"Structural Studies on Thin Polymer Films by X-ray and Neutron

Reflectivity'

Supervisor: Prof KANAYA, Toshiji

24 September 2003

MORIGUCHI, Sakumi

D Sc, Kyoto University

"Improvement and Application of High-resolution Transmission

Electron Microscopy

Supervisor: Prof ISODA, Seiji

24 March 2003

NAGATA, Kazuto

D Sc, Kyoto University

"Studies on the Synthesis and Properties of the Disulfur and Diselenium Complexes of Platinum Utilizing New Bulky

Phosphine Ligands'

Supervisor: Prof TOKITOH, Norihiro

24 March 2003

NAKATA, Norio

D Sc, Kyoto University

"Studies on the Synthesis and Properties of Kinetically Stabilized

Germaaromatic Compounds"

Supervisor: Prof TOKITOH, Norihiro

24 March 2003

NOMURA, Akiko

D Pharm Sc, Kyoto University

"Redesign of the Metal Coordination Sites in the Zinc Finger

Peptides"

Supervisor: Prof SUGIURA, Yukio

24 March 2003

NORISUYE, Kazuhiro

D Sc, Kyoto University

"Development of Analytical Methods for Determining Long-Lived Anthropogenic Radionuclides in Seawater and Analysis of

Sources of Pu Isotopes"

Supervisor: Prof SOHRIN, Yoshiki

24 March 2003

OTSUBO, Tadamune

D Pharm Sc, Kyoto University

"Synthesis and Functions of Homooxacalix[3]arene Derivatives"

Supervisor: Assoc Prof KAWABATA, Takeo

24 March 2003

SAEKI, Tomoyuki

D Eng, Kyoto University

"The Chemistry of Silylenes Intramolecularly Coordinated by

Group 15 and 16 Elements"

Supervisor: Prof TAMAO, Kohei 23 January 2003

SHIRASAKA, Toshiaki

D Eng, Kyoto University

"Photophysical Properties Control of p-Electron Systems

Containing Main-Group Elements'

Supervisor: Prof TAMAO, Kohei

24 March 2003

SUZUKI, Takeshi

D Agr, Kyoto University

"Enzymological Studies of Cold-active Esterases from

Psychrotrophic Bacteria"

Supervisor: Prof ESAKI, Nobuyoshi

24 March 2003

SUZUKI, Tomoki

D Pharm Sc, Kyoto University

"Application as Cellular Carrier of Basic Peptides and

Mechanism of Their Membrane Transmission"

Supervisor: Prof SUGIURA, Yukio

24 March 2003

TAKAISHI, Taigo

D Eng, Kyoto University

"Studies on the Short and Medium Range Structure of Lead-

containing Oxide Glasses"

Supervisor: Prof YOKO, Toshinobu

23 March 2003

TSUTSUMI, Kiyohiko

D Sc, Kyoto University

"Unoccupied Electronic States of Organic Solids Studied by

Inverse Photoemission Spectroscopy'

Supervisor: Prof SATO, Naoki

24 March 2003

YAMAMOTO, Hiroaki

D Agr, Kyoto University

"Studies of Synthesis of Optically Active Alcohols with

Recombinant Whole-cell Biocatalysts'

Supervisor: Prof ESAKI, Nobuyoshi

24 March 2003

YAMANAKA, Rio D Sc, Kyoto University
"Biocatalytic Asymmetric Reduction of Ketones by Photosynthetic Organisms"
Supervisor: Assoc Prof NAKAMURA, Kaoru
24 March 2003

# THE 103RD ICR ANNUAL SYMPOSIUM

# Seminars Meetings and Symposiums

#### THE 103RD ICR ANNUAL SYMPOSIUM

(5 December 2003)

#### **ORAL PRESENTATIONS**

MATUBAYASI, Nobuyuki (Interface Science I) "Properties and Reactions of Supercritical Water"

TOSAKA, Masatoshi (States and Structures III)

"New Aspects in Strain-induced Crystallization of Natural Rubber"

KANAYA, Toshiji (Fundamental Material Properties II)

"Detailed Analysis and Control of Higher Order Structure in Polymer Systems"

SHIMAKAWA, Yuichi (Solid State Chemistry II)

"Functional Oxides: Materials for Magnetic Read Heads and Thermal Radiation Control Devices"

- The ICR Award for Young Scientists -

MURATA, Yasuiiro (Organic Materials Chemistry II)

"Synthesis of Open-Cage Fullerene Derivatives and 100% Encapsulation of a Hydrogen Molecule"

- The ICR Award for Young Scientists -

OHASHI, Yohei (Molecular Biology and Information II)

"Functional Analysis of the *Arabidopsis GLABRA2* Gene That Contributes Root-hair Development through the Modulation of Phospholipid Signaling"

SASAMORI, Takahiro (Bioorganic Chemistry I)

"Studies on Synthesis, Structures, and Properties of Doubly Bonded Systems between Heavier Group 15 Elements"

KATAYAMA, Hiroyuki (International Research Center for Elements Science III)

"Well-Controlled Polymer Synthesis by Transition Metal-Catalyzed Polymerization: Ring-Opening Metathesis Polymerization Using Fischer-type Carbene Catalysts"

KAWABATA, Takeo (Synthetic Organic Chemistry II)

"Asymmetric Alkylation via Memory of Chirality: Mechanism and Its Application to Asymmetric Cyclization"

SAKABE, Shuji (Nuclear Science Research Facility II)

"Ultra-intense Laser Matter Interactions and Their Applications"

UMEDA, Masato (Molecular Biology and Information I) "Approach to Supramolecular Biology"

#### POSTER PRESENTATIONS

W: Laboratory Whole Presentation

I : Laboratory Topic

E: General Presentation

- The ICR Award for Students -

ISHIWATA, Shintaro (International Research Center for Elements Science II)

"High Pressure Synthesis and Crystal Structure of Perovskite BiNiO<sub>3</sub>, and Suppression of A-site Charge Disproportionation by La-substitution"

- The ICR Award for Students -

YAMANISHI, Yoshihiro (Bioinformatics Center I)

"Extraction of Correlated Gene Clusters from Multiple Genomic Data by Generalized Kernel Canonical Correlation Analysis"

#### STATES AND STRUCTURES I

- "Elucidation of Structure-Function Relationship of Protein Molecule by X-ray Crystallographic Analysis"
- © NAKAMATSU, Hirohide; YAMASHITA, Daisuke (Science and Engineering, Waseda University); UDA, Masayuki (Science and Engineering, Waseda University)
  "X-ray Emission Spectra for Fe compounds"

#### STATES AND STRUCTURES II

- W "Recent Studies in the Division of States and Structures II"
- GE MINARI, Takeo
  "Electrical Property and Carrier Transport Process in Single
  Grain Organic Field Effect Transistor"

#### STATES AND STRUCTURES III

- SENOO, Kazunobu; ATSUMI, Kunihiro; MURAKAMI, Syozo; KOHJIYA, Shinzo
  "Ion Conductivity of Uniaxially Stretched High Molecular Weight Poly(ethylene oxide)s"
- © YOSHIOKA, Taiyo; TSUJI, Masaki; KOHJIYA, Shinzo "Morphological Study on Uniaxially Oriented Thin Films of Poly(butylene terephthalate) [PBT]"
- GE FURUTANI, Masahiro; TOSAKA, Masatoshi; KOHJIYA, Shinzo "Effect of Fatty Acids on Strain-induced Crystallization of

#### INTERFACE SCIENCE I

Natural Rubber'

- W "Properties and Reactions of Supercritical Water"
- GE KIMURA, Tomohiro; OKAMURA, Emiko; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru

"NMR Study on the Interactions of Neuropeptides Achatin-I and Met-Enkephalin with Lipid Bilayers"

#### INTERFACE SCIENCE II

- YOSHIDA, Hiroyuki
  "Thin Film Formation by Use of Cluster Beam"
- ASAMI, Koji "Ion Channels Formed in Lipid Bilayers by Alamethicin and Its Analogues"

#### INTERFACE SCIENCE III

We haviors of Dissolved Metals in Hydrothermal Plumes and Diffused Flows at the Suiyo Seamount, Izu-Bonin arc"

#### SOLID STATE CHEMISTRY I

- MIYAKE, Kousaku
  "Magnetic Structures and Magnetoresistance between
  Magnetic Wires"
- © OHKOCHI, Takuo
  "Spin Polarization in Nonmagnetic Layers of Magnetic/
  Nonmagnetic Multilayers"
- GE JIKO, Norihiro "Magnetism of Cr-based Multilayers"

#### SOLID STATE CHEMISTRY IV

- W "Recent Studies in Division of Solid State Chemistry IV"
- © YAMAMOTO, Satomi; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu "Improvement of Water Durability of Organic-inorganic Hybrid Low-melting Glasses Prepared by Non-aqueous Acid-base"
- © ENKHTUVISHIN, Dorjpalam; TAKAHASHI, Masahide; YOKO, Toshinobu "Preparation and Photoelectrochemical Properties of the Sandwich-type Multilayer Tio<sub>2</sub> / MeO<sub>x</sub> / TiO<sub>2</sub> Thin Film Electrodes"
- © SAITO, Masanori; TOKUDA, Yomei; TAKAHASHI, Masahide; YOKO, Toshinobu
  "Local Laser Processing of Organic-inorganic Hybrid Low-Melting Glasses Prepared by Non-aqueous Acid-base Reaction"
- © MASAI, Hirokazu; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu; WATANABE, Hiroshi (Fundamental Material Properties I) "Softening Behavior and Structure of Phenyl/ alkylpolysiloxane Glasses"
- (E) MIZUNO, Megumi; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu "Preparation and Application of Organic-inorganic Hybrid Low-melting Glasses by Non-aqueous Acid-base Reaction"

- © TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu
  "Photoactivated Chemical Reactions and Photorefractivity in Ge-doped SiO<sub>2</sub> Glasses"
- TOKUDA, Yomei; TAKAHASHI, Masahide; YOKO, Toshinobu
  "Time-resolved Photoluminescence Spectra of Ge:SiO<sub>2</sub>
  Glasses"
- ©E ZHANG, Jian; TAKAHASHI, Masahide; TOKUDA, Yomei; YOKO, Toshinobu "Photoluminescence Characteristics of Eu<sup>2+</sup> Doped CaS-Ca<sub>2</sub>S<sub>3</sub> Glass-ceramic Phosphors"

#### FUNDAMENTAL MATERIAL PROPERTIES I

- W "Perspective on Molecular Rheology"
- © KIKUCHI, Toshimitsu "Electric Birefrigence of Amorphous Polymers"

#### FUNDAMENTAL MATERIAL PROPERTIES II

- W "Detailed Structural Analysis and Development of Polymer Materials"
- © YAMANO, Hiroaki; INOUE, Rintaro; MIYAZAKI, Tsukasa; NISHIDA, Koji; KANAYA, Toshiji "Glass Transition of Polymer Thin Films"
- © KONISHI, Takashi; MATSUBA, Go; NISHIDA, Koji; KANAYA, Toshiji "Preparatory Mechanism of Polymer Crystallization"

#### FUNDAMENTAL MATERIAL PROPERTIES III

- KAJI, Hironori; KUSAKA, Yasunari; ONOYAMA, Goro; TSUKAMOTO, Naoki; YAMADA, Tomonori; HORII, Fumitaka
  "Preside Analyses of Structure and Direction in Experience
  - "Precise Analyses of Structure and Dynamics in Functional Materials by Solid-State NMR Spectroscopy"
- GE HIRAI, Asako; HORII, Fumitaka; TSUJII, Yoshinobu (Organic Materials Chemistry I); TSUJI, Masaki (States and Structures III)
  - "AFM Observation of Cellulose Assemblies Produced by Acetobacter Xylinum"

#### ORGANIC MATERIALS CHEMISTRY I

- OHNO, Kohji
  "Precision Design and Application of Organic/Inorganic Hybrid Nanoparticles"
- © KWAK, Yungwan; GOTO, Atsushi; FUKUDA, Takeshi "Kinetic Studies on Organotelluride-Mediated Living Radical Polymerization"
- © YAMANE, Chika
  "Controlled Synthesis of High-Density Polyelectrolyte
  Brushes by Living Radical Polymerization"

#### ORGANIC MATERIALS CHEMISTRY II

- MURATA, Yasujiro; MURATA, Michihisa; KOMATSU, Koichi
  - "Synthesis of Open-Cage Fullerene Derivatives and 100% Encapsulation of a Hydrogen Molecule"
- © UTO, Takayuki; NISHINAGA, Tohru; KOMATSU, Koichi "Reactivity of Benzene and COT Fully Annelated with Bicyclo[2.1.1]hexene"
- (E) YAMAZAKI, Tetsuya; HAN, Aihong; Lin, Jing-Rong; MURATA, Yasujiro; KOMATSU, Koichi "Synthesis and Polymerization of the Propylenedioxy-Substituted Terthiophene-Fullerene Dyads"
- © OGAWA, Kohei; KITAGAWA, Toshikazu; KOMATSU, Koichi
  - "Synthesis and Properties of Azobis(Malachite Green) Dication"

#### SYNTHETIC ORGANIC CHEMISTRY II

- Œ KUSUMOTO, Tomokazu
  - "Visual Recognition using Phenolphthalein Derivertives"
- GE TANAKA, Hiroyuki
  - "Synthesis and Properties of Optically Active Oligonaphthalene Derivatives"
- GE SCHEDEL, Hartmut
  - "Synthesis and Properties of C<sub>2</sub>-Symmetric Chiral Nucleophilic Catalysts"

#### **BIOORGANIC CHEMISTRY I**

- "Synthesis of Novel Organic Compounds Containing Heavier Elements by Taking Advantage of Kinetic Stabilization and the Elucidation of Their Properties"
- © YAMAZAKI, Takayuki; SASAMORI, Takahiro; TAKEDA, Nobuhiro; TOKITOH, Norihiro "Studies on the Synthesis of Novel Heteronuclear Doublebond Compounds between Heavier Group 15 Elements Utilizing Steric Protection"
- E HAMAKI, Hirofumi; TAKEDA, Nobuhiro; TOKITOH, Norihiro
  - "Synthesis of a Novel Bulky Lithium β-Diketiminate Bearing Bulky Substituents and Their Applications to the Synthesis of Complexes of a Group 4 Element"

#### **BIOORGANIC CHEMISTRY II**

- W "Studies of Artificial Zinc Finger Peptides and Membranepermeable Peptides"
- GE NIWA, Miki
  - "Intracellular Delivery of Histidine-tagged Proteins Using Arginine-peptides"

#### **BIOORGANIC CHEMISTRY III**

GE IIDA, Shinya

"Development of a Highly Sensitive Method for Minute Amounts of Nucleic Acids"

GE TAKEHASHI, Masanori "Functional Characterization of Septin 3"

#### MOLECULAR BIOFUNCTION I

- SAITO,Shigeki; MIZUTANI, Masaharu; SAKATA, Kanzo "Characterization of Cytochromes P450 Involved in ABA Catabolism"
- KATO, Masahiro; UNO Tetsuya; HIRATAKE, Jun; SAKATA, Kanzo
  - "Synthesis and Inhibitory Activities of β-Glycosylamidines as β-Glycosidase Inhibitors"

#### MOLECULAR BIOFUNCTION II

- © KWAK, Mi-Sun; MIHARA, Hisaaki; KURIHRA, Tatsuo; YOSHIMURA, Tohru; ESAKI, Nobuyoshi "Studies of tRNA-modifying Enzymes"
- MIHARA, Hisaaki; KURIHARA, Tatsuo; IGARASHI, Motoki; YAMANE, Masahiro; ANO, Kenji; KAZUOKA, Takayuki; YOSHIMURA, Tohru; ESAKI, Nobuyoshi "Studies of Biosynthesis of Iron-Sulfur Clusters"

#### MOLECULAR BIOLOGY AND INFORMATION I

- © TAKEUCHI, Ken-ichi "A Drosophila Cryophilic Mutant, atsugari"
- KATO, Utako "Membrane Lipid Dynamics; Its Role in Cell Morphogenesis"

#### MOLECULAR BIOLOGY AND INFORMATION II

OHASHI, Yohei; OKA, Atsuhiro; AOYAMA, Takashi "Functional Analysis of an *Arabidopsis* Homeobox Gene, *GL2*."

# INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE I

- TAMAO, Kohei; TSUJI, Hayato; SAEKI, Tomoyuki "International Research Center for Elements Science (Organic Main Group Chemistry): Recent Topics in 2003"
- © TSUJI, Hayato; SHIBANO, Yuki; TAMAO, Kohei "Conformation Dependence of the Photophysics of 1,2-Diaryldisilane σ-π Conjugation System"
- © SAEKI, Tomoyuki; Son, Eun-Cheol; MATSUNAGA, Tadafumi; TAMAO, Kohei "Palladium Catalyzed Cross-Coupling Reaction of 1-Aryltriazenes with Areneboronic Acids and Aryltrifluorosilanes"

# INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE II

- TAKANO, Mikio; TERASHIMA, Takahito; AZUMA, Masaki
  - "International Research Center for Elements Science (Advanced Solid State Chemisitry): Recent Topics in 2003"

- © YAMAMOTO, Shinpei; TAKANO, Mikio "Nanocomposite Magnets Prepared by Core-shell Nanoparticles"
- © BELIK, Alexei A.; AZUMA, Masaki; TAKANO, Mikio "Low-dimensional Magnets among Cu-containing Phosphates and Vanadates"
- © KAN, Daisuke; TERASHIMA, Takahito; TAKANO, Mikio; YAMANAKA, Akio (Chitose Institute of Science and Technology)

  "Preparation and Optical Properties of Single Crystalline

"Preparation and Optical Properties of Single-Crystalline CaCuO<sub>2</sub> Thin Film"

GE ISHIWATA, Shintaro

"High Pressure Synthesis, Structure Analysis and Lasubstitution Effect of a Novel Perovskite BiNiO<sub>3</sub>"

#### **BIOINFORMATICS CENTER I**

- W "The Ortholog Clustering (KEGG/OC) using KEGG/SSDB"
- (Correlation Analysis of Multiple Types of Genomic Data"

#### **BIOINFORMATICS CENTER II**

LT UEDA, Nobuhisa

"Algorithms for Classifying Proteins from Sequences and Inferring Protein-protein Interactions"

#### **BIOINFORMATICS CENTER**

Contributed Chair

- Proteome Informatics (SGI Japan) -
- AOKI, Kiyoko F.; YAMAGUCHI, Atsuko "Algorithms and Statistical Analysis of Structural and Functional Properties of Carbohydrate Chains"

#### **BIOINFORMATICS CENTER**

- Bioinformatics Training Unit -
- © DAIYASU, Hiromi; KUMA, Keiichi; TOH, Hiroyuki "Expansion of the New Photolyase / Cryptochrome Subfamily, DASH"

#### NUCLEAR SCIENCE RESEARCH FACILITY I

- TANABE, Mikio; SHIRAI, Toshiyuki; IKEGAMI, Masahiro; TONGU, Hiromu; NODA, Akira "Design of Deflection Electrodes in the Bending Magnet for Zero Dispersion"
- ©E TONGU, Hiromu "Design of S-LSR Vacuum System"
- TAKEUCHI, Takeshi
  "Magnetic Field Measurement of S-LSR Quadrupole Magnets"

#### NUCLEAR SCIENCE RESEARCH FACILITY II

HASHIDA, Masaki; SAKABE, Shuji "Intense Short Pulse Laser Ablation of Metals: Formation of Nanostructure"

#### **SEMINARS**

Prof AJAYAGHOSH, Ayyappanpillai

Regional Research Laboratory (CSIR), India

"π-Extended Squaraines as Intrinsic Conductors and Cation Sensors"

17 September 2003

Mr ALIOTO, Tyler

Department of Molecular and Cell Biology, University of California, Berkeley, USA

"Characterization of the Odorant Receptor C Family in Zebrafish"

2 June 2003

Prof BARTHEL, Josef

University of Regensburg, Germany

"The Role of Ion Aggregation in Physical Properties of Electrolytes Solutions"

16 October 2003

Prof BÄUERLE, Peter

Department Organic Chemistry II, University of Ulm, Germany "Combinatorial Organic Materials Research (COMR): A Faster Route to Organic Materials"

10 November 2003

Prof BROCHARD-WYART, Francoise

University P et M Curie, France

"Hydroplaning of Cars'

2 June 2003

Prof BULANOV, Sergei V.

Kansai Research Establishment, JAERI, Kyoto, Japan / Institute of General Physics, Russian Academy of Sciences, Moscow, Russia

"Interaction of Charged Particles with Ultra Strong Electromagnetic Waves in the Radiation Dominant Regime" 11 December 2003

Prof CERVANTES, Jorge A.

University of Guanajuato, Mexico

"Alkoxysilanes: Synthesis and Applications to Architectural Conservation"

16 October 2003

Prof DE GENNES, Pierre-Gilles

College de France, France

"Phase Transitions of Nematic Rubbers"

2 June 2003

Dr DEVOLDER, Thibaut

CNRS-Université Paris-Sud, Orsay, France

"Irradiation-Induced Magnetic Property Modifications: Basic Phenomena, Nanostructure Fabrication and Potential Applications"

18 February 2003

Dr DOWDY Steven F.

Howard Hughes medical Institute, UCSD School of Medicine, La Jolla CA, USA

"Delivery of Novel Anti-Cancer Therapeutics and Mechanism of Protein Transduction"

23 June 2003

Dr GLOTTER, Alexandre

Laboratoire de Physique des Solides, CNRS, France

"Implementing Spectral Deconvolution into Spectrum-imaging Mode: A New Step towards Combined High Spatial and Energy-resolution EELS"

21 November 2003

Dr GRIESER, Manfred

Max-Planck-Institut für Kernphysik, Heidelberg, Germany

"Low Energy Storage Rings for Molecules, Heavy Ions and Antiprotons"

13 May 2003

Prof HALEY, Michael M.

Department of Chemistry, University of Oregon, USA

"Chemistry of Metallabenzenes and Valence Isomers: New Ligands, New Metals, New Insights"

1 October 2003

Prof HALLDORSON, Magnus

Department of Computer Science, Faculty of Engineering,

University of Iceland, Iceland

"Design of a Marker Set for a Whole Genome Scan for Cancer"

21 April 2003

Prof HUMERES, Eduardo

Department of Chemistry, Universidade Federal de Santa

Catarina, Brasil

"Supermolecular Catalysis Induced by Polysaccharides"

6 October 2003

Prof INOUE, Jun-ichiro

Graduate School of Engineering, Nagoya University, Japan

"Magnetoresistance in Exchange-Spring Multilayers with Twisted Spin Structures (Theories)"

12 May 2003

Prof INOUE, Jun-ichiro

Graduate School of Engineering, Nagoya University, Japan

"Recent Topics on Spintronics'

9 June 2003

Prof INOUE, Jun-ichiro

Graduate School of Engineering, Nagoya University, Japan

"Magnetism - From Fundamentals to Spintronics I"

2 October 2003

Prof INOUE, Jun-ichiro

Graduate School of Engineering, Nagoya University, Japan

"Magnetism - From Fundamentals to Spintronics II"

16 October 2003

Prof INOUE, Jun-ichiro

Graduate School of Engineering, Nagoya University, Japan

"Magnetism - From Fundamentals to Spintronics III"

23 October 2003

Prof ISSIKI, Kenji

Kochi Women's University, Kochi, Japan

"Properties of Muroto Ocean Deep Water on the Basis of Trace

Metals"

6 December 2003

Dr IWASE, Hiroki

Institute of Materials Structure Science, High Energy Accelerator Research Organization, Japan

"Studies of Biomembranes Using the Neutron and X-ray Scattering Methods"

12 December 2003

#### Dr KAPIN, Valeri

National Institute of Radiological Sciences, Japan / Moscow Engineering Physics Institute, Russia

"The Compact Linac (IH linac) for the Medical Accelerator" 19 September 2003

#### Prof KIM, Yong Hae

Korean Advanced Institute of Science and Technology (KAIST), Korea

"Asymmetric Synthesis by Dual Enantioselective Control" 25 February 2003

#### Prof KIMURA, Tsunehisa

Faculty of Engineering, Tokyo Metropolitan University, Japan "Material Processing by Using a Magnetic Field" 30 January 2003

#### Assoc Prof KOWALEWSKI, Tomasz

Carnegie Mellon University, USA

"Nanostructured sp<sup>2</sup> Carbon Materials Derived from Well-Defined Block Copolymers" 16 May 2003

#### Prof LAMMERTSMA, Koop

Vrije University, Amsterdam, Netherlands

"Organophosphorus Reagents-design, Properties, and Applications"

20 February 2003

#### Prof LAUPRETRE, Francoise

Laboratoire de Physico-Chimie Structurale et Macromoléculaire, Paris XII-Val de Marne University, France

"NMR Investigation of the Molecular Organization of Complex Polymer Systems"

13 May 2003

#### Prof LEE, Myong Euy

Department of Chemistry, Yonsei University, Korea "Disilanols: Syntheses, Structures and Reactivities" 16 October 2003

#### Prof LIU, Hung-wen

Division of Medicinal Chemistry, College of Pharmacy, and Department of Chemistry and Biochemistry, University of Texas, LISA

"The Mechanistic Studies of UDP-galactopyranose Mutase: an Unusual Role of FAD in Enzyme Catalysis" 20 October 2003

#### Prof MATYJASZEWSKI, Krzysztof

Carnegie Mellon University, USA

"Mechanisms of Atom Transfer Radical Polymerization" 16 May 2003

#### Prof MESHKOV, Igor N.

Joint Institute for Nuclear Research, Dubna, Russia

"Electron Cooling Studies and Applications at Joint Institute for Nuclear Research"

7 May 2003

#### Assoc Prof MITANI, Seiji

Institute for Materials Research, Tohoku University, Japan "Tunneling Magnetoresistance in Granular Thin Films - From

Basics to Applications - III" 14 January 2003

#### Assoc Prof MITANI, Seiji

Institute for Materials Research, Tohoku University, Japan "Perpendicular Magnetoresistance in Co/Gd Multilayers with Twisted Spin Structures (Experiments)" 12 May 2003

#### Dr NIERENGARTEN, Jean-François

Institut de Physique et Chimie des Matériaux de Strasbourg, Groupe des Matériaux Organiques, Université Louis Pasteur et CNRS, France

"Oligophenylenevinylene Oligomers: Versatile Building Blocks for Supramolecular Chemistry and Materials Science Applications"

26 November 2003

#### Prof OGAWA, Kazufumi

Faculty of Engineering, Kagawa University, Takamatsu, Japan "Applications of Chemisorbed Monomolecular Films: Attempts to Realize Molecular Wiring" 17 January 2003

#### Dr PANKHURST, Quentin A.

University College London, London, UK
"Exchange Pinning in Core-Shell Nanoparticles"
3 March 2003

#### Assoc Prof PILON, Marinus

Biology Department, Colorado State University, USA "Metal Cofactor Assembly and Homeostasis in Plastids" 4 November 2003

#### Assoc Prof PILON-SMITS, Elizabeth

Biology Department, Colorado State University, USA

"Studying Selenium Metabolism in Plants – A Biotechnological Approach"

4 November 2003

#### Dr REISTAD, Dag

The Svedberg Laboratory, Uppsala, Sweden "Status of Svedberg Laboratory in Uppsala and Future Plans" 16 May 2003

#### Prof RICHARDS, Nigel G. J.

Department of Chemistry, University of Florida, USA "Structure-Based Discovery of Inhibitors of Human Asparagine Synthetase"

4 July 2003

#### Prof ROTH, Markus

Technische Universität Darmstadt, Darmstadt, Germany "Laser Ion Production and its Beam Quality" 19 February 2003

#### Prof RUBIN, Yves

Department of Chemistry and Biochemistry, University of California, Los Angeles, USA

"Chemistry of  $C_{60}$  and Approaches to Endohedral Metallofullerenes"

1 October 2003

#### Prof SCOTT, Lawrence T.

Merkert Chemistry Center, Boston College, USA

"Chemical Methods for the Rational Synthesis of Fullerenes and Carbon Nanotubes"

15 November 2003

#### Dr SHCHAGIN, Alexander V.

Hiroshima University, Hiroshima, Japan / Kharikov Institute of Physics and Technology, Kharkov, Ukraine "Investigation of Properties of Properties V ray Padiation"

"Investigation of Properties of Parametric X-ray Radiation" 10 February 2003

#### Prof SHEVELKO, Viatcheslav P.

National Institute of Radiological Sciences, Chiba, Japan / P.N. Lebedev Physical Institute, Moscow, Russia "Target-density Effects in Electron-Capture Processes" 16 October 2003

#### Prof SHINMYOZU, Teruo

Institute for Materials Chemistry and Engineering, Kyushu University, Japan

"Synthesis, Structure, and Photoreaction of [3] Superphanes" 26 July 2003

#### Prof SHUBIN, Vyacheslav G.

Novosibirsk Institute for Organic Chemistry, Russia "Long-Lived Cationic Complexes: Structure and Reactivity" 15 December 2003

#### Dr SOLLADIÉ, Nathalie

Laboratoire d'Electrochimie et de Chimie Physique du Corps Solide, Université Louis Pasteur et CNRS, France "Structure-Reactivity Correlations in Extended Multi-Porphyrinic Architectures" 26 November 2003

#### Dr SYRESIN, Evgeny

Joint Institute for Nuclear Research, Dubna, Russia "LSR Electron Cooler Simulation" 9 January 2003

#### Dr SYRESIN, Evgeny

Joint Institute for Nuclear Research, Dubna, Russia "Ion Beam Stability at Cooling Stacking Injection" 29 August 2003

Prof TANABE, Tetsumi KEK, Ibaraki, Japan "Electrostatic Storage Ring" 13-14 February 2003

#### Prof ULANSKI, Jacek

Technical University of Lodz, Poland "Low Frequency Raman Scattering in Polymers" 21 November 2003

Assoc Prof UTTAPAP, Dudsadee King Mongkut's University of Technology, Thailand "Properties of Edible Canna Starches"

11 November 2003

Prof VLASSOPOULOS, Dimitris FORTH and University of Crete, Greek "Control of the Rheological Behavior of Colloidal Star Polymers" 20 March 2003

Prof WATANABE, Junji Tokyo Institute of Technology, Tokyo, Japan "Banana-Shaped Liquid Crystal" 6 June 2003

Dr WATSON, William P.

Syngenta Central Toxicology Laboratory, UK

"Molecular Toxicology of Dienes" 10 October 2003

#### Prof WONG, Henry N. C.

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

"The Quest of Non-natural Molecules: Hydroxytetraphenylenes and Pentacenes"

21 November 2003

#### Dr YAMAZAKI, Yoshishige

Japan Atomic Energy Research Institute, Japan

"Design Principles of JPARC Accelerator and Construction Status"

10 June 2003

#### MEETINGS AND SYMPOSIUMS

# The 9th International Seminar on Elastomers (ISE 2003) by Institute for Chemical Research, Kyoto University

Organized by KOHJIYA, Shinzo 2-4 April 2003 (Kyoto, Japan)

# Minisymposium: Progress in Organic Silicon Chemistry

Organized by SATO, Naoki; TOKITOH, Norihiro 19 June 2003

#### MATSUMOTO, Hideyuki

Gunma University

"Syntheses and Properties of Silicon-Based Condensed Polycyclic Molecules — Toward Fabrication of Si-Based Molecules of High Originality"

#### NISHINAGA, Tohru

Kyoto University

"Properties of Silicon Cations Embedded in  $\pi$ -Conjugated Systems"

#### TAKEDA, Nobuhiro

Kyoto University

"Creation of Novel Silicon-Active Chemical Species by Making Use of Bulky Substitutents and Their Reactivities"

#### HIRATSUKA, Hiroshi

Gunma University

"Photophysics and Photochemistry of Organic Silicon Compounds"

#### TSUJI, Hayato

Kyoto University

"Conformation and Optical Properties of Silicon  $\sigma$ -Conjugated Systems"

## 8th Symposium of the Society of Silicon Chemistry Japan

Organized by TOKITOH, Norihiro 17-18 October 2003 (Kyoto)

#### **Plenary Lecture**

Prof ISHIKAWA, Mitsuo

Department of Chemistry and Bioscience, Kurashiki University of Science and the Arts, Japan

"Synthesis and Thermal Properties of Silacyclobutenes"

#### **Invited Lectures**

Prof KAWAKAMI, Yusuke

School of Materials Science, Japan Advanced Institute of Science and Technology, Japan

"Elucidation of Stereochemistry of Asymmetric Silicon Centers by the Aid of Optically Active Silicon Compounds" Prof LEE, Myong Euy

Department of Chemistry, Yonsei University, Korea

"Syntheses and Reactivities of Stable Halosilylenoids, (Tsi) $X_2$ SiM (Tsi = C(SiMe<sub>3</sub>)<sub>3</sub>, X = Br, Cl, M = Li, K)"

#### Dr IWAMOTO, Takeaki

Department of Chemistry, Graduate School of Science, Tohoku University, Japan

"Synthesis, Structure, and Properties of Stable Conjugated Disilenes"

#### Mr USHIO, Yoshito

Electronics Industry S&T, Dow Corning Toray Silicone Co., Ltd., Japan

"Development of Silicone Elastomer Film Adhesive"

#### Prof CERVANTES, Jorge

Chemistry Department, University of Guanajuato, Mexico "Silicon Chemistry and Technology, Experiences in Building –up Research Program"

#### Dr SANJI, Takanobu

Chemical Resources Laboratory, Tokyo Institute of Technology, Japan

"How to Make Polysilanes with Controlled Structure"

#### Dr IMAI, Takafumi

Pacific R&D Center, GE Toshiba Silicones Co., Ltd., Japan "Silicone Industry – the Present and the Future"

#### Prof SEKIGUCHI, Akira

Department of Chemistry, University of Tsukuba, Japan "The Power of 'Silyl-Trick': Silyl-Substituted Tetrahedrans and Stable Heavier Group 14 Element Radicals"

#### Prof TAKAHARA, Atsushi

Institute of Materials Chemistry and Engineering, Kyushu University, Graduate School of Engineering, Kyushu University, Japan

"Two-dimensional Surface Property Control of Organosilane Nanofilms"

In addition, 88 posters were presented.

# The 21st Century COE-ICR Research Seminar on "Organic Thin Films"

Organized by SATO, Naoki; ISODA, Seiji; UMEMURA, Junzo; YOSHIDA, Hiroyuki 7-8 November 2003

#### OZAKI, Hiroyuki

Tokyo University of Agriculture and Technology

"Formation, Characterization, Superstructure Fabrication of Organic Ultra-Thin films"

#### HASEGAWA, Takeshi

Nihon University

"New Analytical Method of Structural Anisotropies in Organic Thin Films with Infrared Spectroscopy"

#### KIMURA, Shunsaku

**Kyoto University** 

"Measurements of Orientation of Helical Peptides at the Interfaces"

#### IWAMOTO, Mitsumasa

Tokyo Institute of Technology

"Examination of Dielectric Polarization Behaviors of Organic Molecular Films with their Maxwell Current, Surface Potential and Second Harmonic Generation Measurements"

#### ISHII, Hisao

Tohoku University

"Charging and Polarization Behaviors in Organic Thin Films and at their Interfaces"

#### MUNAKATA, Toshiaki

The Institute of Physical and Chemical Research (RIKEN)

"Development of Photoemission Microspectroscopy using Femtosecond Lasers"

#### YOSHIDA, Hiroyuki

Kyoto University

"Observation of Electronic Structures of Unoccupied States in Organic Thin Films using Inverse Photoemission Spectroscopy — Correlation with Polymorphism in the Case of Lithium Phthalocyanine"

#### YAMADA, Hirofumi

Kyoto University

"Examination of Organic Molecular Materials with Atomic Force Microscopy in the Dynamic Mode"

#### OGAWA, Kazufumi

Kagawa University

"Fundamentals and Applications of Chemisorbed Monomolecular Films"

#### YANAGI, Hisao

Kobe University

"Fabrications and Properties of Organic Low-Dimensional Structures in the Nano- to Meso-scopic Scales"

#### HOSHINO, Akitaka

Kyoto University

"Variety in the Structure of Organic Epitaxial Films Based on Lattice Matching at the Interface"

#### SHIMADA, Toshihiro

The University of Tokyo

"Studies of Organic Thin Films using Surface Spectroscopy of FET Structures and Pulsed Molecular Beams"

#### KURATA, Hiroki

Kyoto University

"Structural Analyses of Organic Thin Films with Electron Spectromicroscopy"

Kyoto University Alliance for Chemistry 21st Century COE Program, Elucidation of Nano Structures and Properties of Elastomeric Materials by Institute for Chemical Research, Kyoto University

Organized by KOHJIYA, Shinzo 14 November 2003 (Kyoto, Japan)

#### 44th Meeting on Glass and Photonics Materials

Organized by YOKO, Toshinobu 20-21 November 2003(Kyoto)

COE Program for the 21st Century "Kyoto University Alliance for Chemistry", ICR Symposium on Structural Organic Chemistry — Development of the Chemistry of  $\pi$ -Conjugated Systems

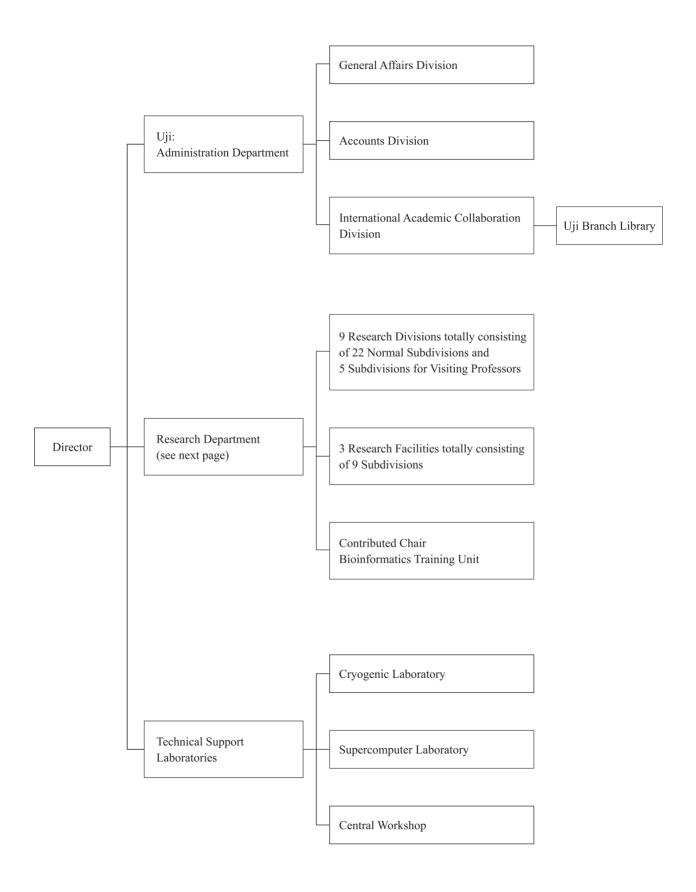
Organized by KITAGAWA, Toshikazu 1-2 December 2003 (ICR, Kyoto)

#### Workshop for Design of Cooler Ring, S-LSR

Organized by NODA, Akira (Kyoto University) and NODA, Koji (National Institute for Radiological Sciences) 2-5 December 2003 (Kyoto)

# ORGANIZATION AND STAFF

## INSTITUTE FOR CHEMICAL RESEARCH, KYOTO UNIVERSITY



# **RESEARCH DIVISION**

(As of 31 December 2003)

	Research Division	Subdivision(Laboratory)	Professor	Associate Professor	Instructor	Associate Instructor /Technician
-		I . Atomic and Molecular Physics —	— HATA, Yasuo —	— ITO, Yoshiaki –	NAKAMATSU, Hirohide FUJII, Tomomi	
	States and Structures —	II. Electron Microcopy and Crystal Chemistry —	— ISODA, Seiji —	— KURATA, Hiroki –	OGAWA, Tetsuya NEMOTO, Takashi	– MORIGUCHI, Sakumi
		III. Polymer Condensed States —	— KOHJIYA, Shinzo —	— TSUJI, Masaki –	TOSAKA, Masatoshi SENOO, Kazunobu	
		I. Solutions and Interfaces —	NAKAHARA, Masaru UMEMURA, Junzo	— MATUBAYASI, Nobuyuki —	OKAMURA, Emiko WAKAI, Chihiro	
	— Interface Science —	II. Molecular Aggregates —	— SATO, Naoki —	— ASAMI, Koji –	KITA, Yasuo YOSHIDA, Hiroyuki	
		III. Hydrospheric Environment Analysis —	— SOHRIN, Yoshiki —	— UMETANI, Shigeo –	SASAKI, Yoshihiro	NORISUYE, Kazuhiro MINAMI, Tomoharu
		I . Artificial Lattice Alloys	— (to be filled)	[Adjunct Assoc Prof] ONO, Teruo	, ,	,
	— Solid State Chemistry –	II. Advanced Inorganic Synthesis —	— SHIMAKAWA, Yuichi —	— (Vacancy) —	IKEDA, Yasunori	
		IV. Amorphous Materials	— YOKO, Toshinobu —	— TAKAHASHI, Masahide —	— TOKUDA, Yomei —	- ENKHTUVSHIN, Dorjpalam
		I . Molecular Rheology —	WATANABE, Hiroshi	— INOUE, Tadashi —	—— MATSUMIYA, Yumi ——	- OKADA, Shinichi
	Fundamental Material _ Properties	II. Polymer Materials Science —	— KANAYA, Toshiji —	— (Vacancy) —	NISHIDA, Koji	
		III. Molecular Dynamic Characteristics —	— HORII, Fumitaka —	— KAJI, Hironori –	— HIRAI, Asako —	- OHMINE, Kyoko
	Organic Materials _	I . Polymeric Materials —	— FUKUDA, Takeshi —	— TSUJII, Yoshinobu –	OHNO, Kohji GOTO, Atsushi	
·	Chemistry	II. Organic Structural Chemistry —	— KOMATSU, Koichi —	— KITAGAWA, Toshikazu —	NISHINAGA, Tohru MURATA, Yasujiro	
	Synthetic Organic _ Chemistry	— II. Fine Organic Synthesis —	— (to be filled) —	— KAWABATA, Takeo –	— TSUBAKI, Kazunori	- TERADA, Tomoko
		I. Organoelement Chemistry	— TOKITOH, Norihiro —	— NAKAMURA, Kaoru –	KAWAI, Yasushi TAKEDA, Nobuhiro SASAMORI, Takahiro	– HIRANO, Toshiko
	Bioorganic Chemistry —	II. Bioactive Chemistry —	— SUGIURA, Yukio —	— FUTAKI, Shiroh –	— IMANISHI, Miki	
		III. Molecular Clinical Chemistry —	— UEDA, Kunihiro —	— TANAKA, Seigo		
		I. Chemistry of Molecular Biocatalysts —	— SAKATA, Kanzo —	— HIRATAKE, Jun –	MIZUTANI, Masaharu SHIMIZU, Bun-ichi	
	— Molecular Biofunction –	II. Molecular Microbial Science —	— ESAKI, Nobuyoshi —	— KURIHARA, Tatsuo –	— MIHARA, Hisaaki	
Director	Molecular Biology	I. Biopolymer Structure —	— UMEDA, Masato —	— (Vacancy) —	TAKEUCHI, Kenichi KATO, Utako	
TAKANO, Mikio	and Information -	II. Molecular Biology —	— OKA, Atsuhiro —	— SUGISAKI, Hiroyuki – — AOYAMA, Takashi –	[Suspension] SAKAI, Hiroe	- OHASHI, Yohei - YASUDA, Keiko
		I . Organic Main Group Chemistry —	— TAMAO, Kohei —	— (Vacancy) —	TSUJI, Hayato SAEKI, Tomoyuki	·
	International Research Center for Elements _	— II. Advanced Solid State Chemistry —	— TAKANO, Mikio —	— TERASHIMA, Takahito –	—— AZUMA, Masaki ——	- YAMAMOTO, Shinpei
	Science [Section Head:TAMAO, Kohei]	III. Organotransition Metal Chemistry —	— OZAWA, Fumiyuki —	— (Vacancy) —	KATAYAMA, Hiroyuki	
		IV. Photonic Elements Science —	KANEMITSU, Yoshihiko (1 Jan. 2004~)	— (Vacancy)		
		I. Bioknowledge Systems —	— KANEHISA, Minoru —	— GOTO, Susumu –	KAWASHIMA, Shuichi HATTORI, Masahiro	
	Bioinformatics Center [Section Head:KANEHISA, Minoru]	II. Biological Information Network —	— AKUTSU, Tatsuya —	— (Vacancy) —	— UEDA, Nobuhisa	
		III. Pathway Engineering	— (Vacancy)	— (Vacancy)		
	— Contributed Chair -	Proteome Informatics (SGI Japan) —		— MAMITSUKA, Hiroshi –	—— YAMAGUCHI, Atsuko	
	- Bioinformatics Center -	Bioinformatics Training Unit —	— TOH, Hiroyuki —	— KUMA, Keiichi –	DAIYASU, Hiromi ICHIHARA, Hisako	
	— Supercomputer Laboratory —		[Section Head] KANEHISA, Minoru			
	Nuclear Science	I. Particle and Photon Beams	— NODA, Akira —	— IWASHITA, Yoshihisa –	—— SHIRAI, Toshiyuki ——	– TONGU, Hiromu
	Research Facility [Section Head:NODA, Akira]	II. Beams and Fundamental Reaction —	SAKABE, Shuji MATSUKI, Seishi	— (Vacancy) —	—— HASHIDA, Masaki	
	- Visiting Division					
		— G. Solid State Chemistry —	— INOUE, Jun-ichiro —	— YAMANAKA, Akio		
		G. Fundamental Material Properties	— YABUKI, Kazuyuki —	— SATO, Takaya		
		G. Synthetic Organic Chemistry	— YAMAMOTO, Yohsuke —	- SUGIO, Shigetoshi		
		G. International Research Center for Elements Science	— TATSUMI, Kazuyuki ——	— YANO, Yoshihiko		
		G. International Research Center for Elements Science (Foreign Guest Laboratory)	— LIU, Yunqi (5 Jan 4 A	pr. 2004)		
	Low Temperature Laboratory					- KUSUDA, Toshiyuki
	— Central Workshop —					_ IMANISHI, Katsumi KAZAMA, Ichiro

(G : Laboratory for Visiting Professor)

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