
ICR ANNUAL REPORT 2002



**Institute for Chemical Research
Kyoto University**
Volume 9

Preface



It is a great pleasure for us to publish the ICR Annual Report for 2002 with the cover page newly designed so that it shows the activity of our institute more vividly than before.

In 2002 we underwent several important organizational changes. The establishment of a new research center named "Research Center for Elements Science" has been officially approved. Starting in April of 2003, this center will consist of four laboratories and two guest-laboratories and cover the fields of organic synthesis, inorganic synthesis, coordination chemistry, and photo-quantum nanochemistry.

The Bioinformatics Center's Laboratory of Proteome Informatics (donated by SGI Japan) started its activity to develop novel computational techniques to elucidate systematic principles of protein interactions in April 2002. Another new laboratory named the "Bioinformatics Training Unit," which is led by a guest-professor TOH Hiroyuki, was organized in October. This new unit will develop methodologies to extract biological knowledge from sequence and structure data of individual genes and proteins, genome data, and expression profile data. This group will also analyze the data of molecular biology from the evolutionary viewpoint in order to obtain fundamental biological knowledge.

We have appointed three new full professors. Professor HATA Yasuo, Professor WATANABE Hiroshi, and Professor KANAYA Toshiharu were promoted to succeed the professorship, respectively, of the Laboratory of Atomic and Molecular Physics (April 2002), the Laboratory of Molecular Rheology and the Laboratory of Polymeric Materials Science (January 2003).

Thus ICR will be expanded to a system of 9 divisions and 3 affiliated research centers in April 2003, consisting of 31 laboratories and 5 guest-laboratories in total. At the

present time, 25 full professors, 21 associate professors, and 43 instructors work in the ICR, and about 220 graduate students and 20 foreign researchers study at the ICR.

A project named "Kyoto University Alliance for Chemistry (Chemistry for Materials Conversion)" started in October, in which the Graduate School of Science, Graduate School of Engineering, and ICR are involved. This project was selected in the field of Chemistry/Materials Science of the 21st Century Center-of-Excellence Program conducted by MEXT. The project aims at establishing a world-leading center for research and education in the field of the chemistry for materials conversion. This interdisciplinary research group will explore the control of chemical bonds, reactions, structures, and functionality of materials.

The organization of national universities must and will be significantly changed by transformation into co-operate bodies 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.

January 2003

A handwritten signature in black ink that reads "Mikio Takano".

Mikio Takano
Director

Institute for Chemical Research Activities

The 102nd ICR Annual Symposium

"The 102nd ICR Annual Symposium" was held at the Joint Research Laboratory on December 6, 2002. The major aim of the symposium is to promote the exchange of information among the members of the institute and to make the achievements of ICR available to the public. ICR scientists presented their research findings by oral and poster presentations. The research involved is at the forefront of science, particularly in the field of chemistry.



The poster session provides the best opportunity for understanding of the research activities of participants. Unlike oral presentations, personal contact between scientists, in front of a poster, often encourages an enthusiastic discussion of results and stimulates the development of new ideas for future research.

Symposium of Graduate Students

ICR also encourages and supports the training of graduate students. The "Symposium of Graduate Students" is intended to encourage graduate students at ICR to present their research findings and to gain experience in discussing their research with other scientists. Doctoral candidates present their findings in oral presentations, while Master's candidates report in a poster presentation.



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Abbreviations 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		



TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Key to headline in the columns

RESEARCH DIVISION
- Laboratory (Subdivision)* -

* See also "ORGANIZATION AND STAFF"
on pages 110 and 111.

States and Structures

- Atomic and Molecular Physics -

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SHIGEOKA, Nobuyuki (D3)
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Wonkwang University, Korea, 6–12 March, 2002, Korea, 27 September–1 October, 2002
Institute of Nuclear Physics of the Hungarian Academy of Science, Hungary, 25 October, 2002

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 2002)

Presentations

Structure-based analysis of functional sites of thermostable aspartase, Fujii T, Sakai H, Kawata Y (Tottori), Hata Y, XIX Congress and General Assembly of the Int. Union of Crystallography, 7 - 10 August.

Crystal structures of pokeweed lectins, Hayashida M, Fujii T, Ishiguro M (Kyushu), Hata Y, Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 26 March, Annual Meeting, Prot. Sci. Soc. Jpn., 14 June, Kyushu Symp. on Struct. Funct. Prot. Enzy., 18 July, XIX Congress and General Assembly of the Int. Union of Crystallography, 12 - 15 August, Annual Meeting, Jpn. Biochem. Soc., 16 October, Annual Meeting, Crystallogr. Soc. Jpn., 11 December.

Role of electrostatic interactions in myosin filament formation, Akutagawa T, Hata Y, Ooi T and Katayama E (Tokyo), Annual Meeting, Biophys. Soc. Jpn., 4 November.

X-ray emission spectroscopy around the threshold in 3d and heavy elements, Ito Y, Fukushima S (NIMS), 6th Forum on Superionic Conductor Physics, 15 - 16 May, 19th Int. Conf. on X-ray and Inner-shell Processes, 24 - 28 June, Int. Seminar on Photoionization in Atom, 19 - 20 August, 28th Symposium on Solid State Ionics, 13 - 15 November.

The Mechanism of X-ray emission satellite excited by SR, Vlaicu A. M. (NIMS), Ito Y, Shigeoka N, Oohashi H, Fukushima S (NIMS), Spring Meeting, The Spectro. Soc. Jpn., 16 - 17 May, 19th Int. Conf. on X-ray and Inner-shell

Processes, 24 - 28 June, Int. Seminar on Photoionization in Atom, 19 - 20 August. Int. Conf. on the Application and Industry, CAARI 2002, 12 - 16 November.

Grants

Hata Y, Structural investigations of 2-oxo acid:ferredoxin oxidoreductases from archaea, Grant-in-Aid for Scientific Research on Priority Areas (A), 1 April 2001 - 31 March 2003.

Hata Y, X-Ray crystal structure analyses of functional proteins, Grant of Rice Genome Project PR-2202, MAFF, JAPAN, 1 April 2000 - 31 March 2003.

Hata Y, Protein-engineering studies on the unique conformations and the expression mechanism of function of pokeweed lectins, 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.

Ito Y, For attendance at the international seminar, the Kyoto University Foundation, 2002, Izumi Science and Technology Foundation, 2002.

X-ray crystal structure analysis of pokeweed lectins, PL-D1 and PL-D2

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. Of these lectins, PL-D is the smallest one consisting of two chitin-binding domains, each of which has four S-S bridges and the putative saccharide-binding site. PL-D has two isomers of PL-D1 and PL-D2. PL-D1 comprises 84 amino acid residues and has a molecular mass of 9,317, while PL-D2 has an identical sequence to that of PL-D1 except for the lack of the C-terminal two residues Leu83-Thr84. The crystal structures of PL-D1 and PL-D2 have been solved by the molecular replacement method and refined up to 1.6 Å and 1.5 Å resolutions with the R-factors of 17.5% and 17.6%, respectively. Both PL-Ds have two saccharide-binding sites which are located on one side of the molecule. The relative orientation of the domains is different by 10° in inclination between PL-D1 and PL-D2. The elongated C-terminal two residues in PL-D1 was not observed in the present crystal structure, indicating the flexibility of the region. The C-terminal

Li K-edge x-ray absorption spectra for lithium compounds

X-ray absorption spectroscopy is expected for a useful method to detect local structure changes and to analyze local quantum structures around Li atoms in various lithium compounds which are studied for developing rechargeable batteries with high capacity.

We have obtained Li K-edge x-ray absorption spectra by electron yield method suitable for the low energy of Li absorption [1]. The results were compared with theoretical spectra and characterized using wave functions which were derived by combination of the molecular orbital and L^2 methods (Fig. 1).

Lithium metal, halides, chalcogenides, oxoacid salts, etc. were studied. Local structure sensitive features and spatial regions of core excitons were revealed. Most of the peaks were assigned to scattering of excited electrons and the characteristic array of the scattering atoms was illustrated for each peak.

1. J. Tsuji et al., *X-ray Spectrometry*, **31**, 319 (2002).

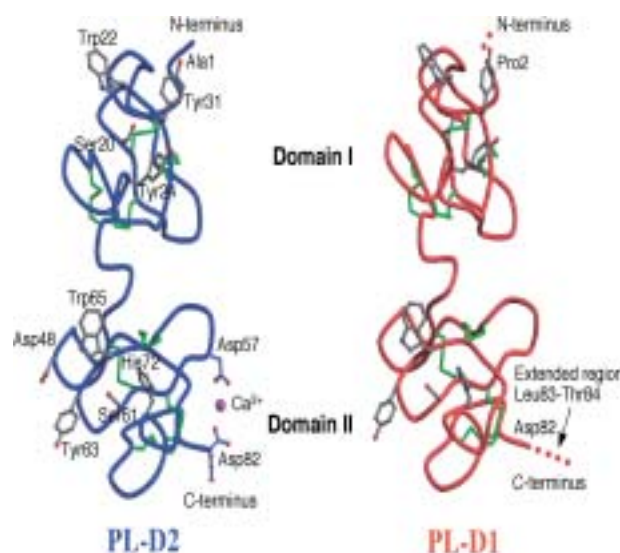


Figure 1. Perspective structures of PL-D1 and PL-D2

α -carboxyl group of PL-D2 binds the Ca^{2+} ion which is coordinated by the β -carboxyl group of Asp57, three water molecules, and the β -carboxyl group of Asp48 from the neighboring molecule in the crystal.

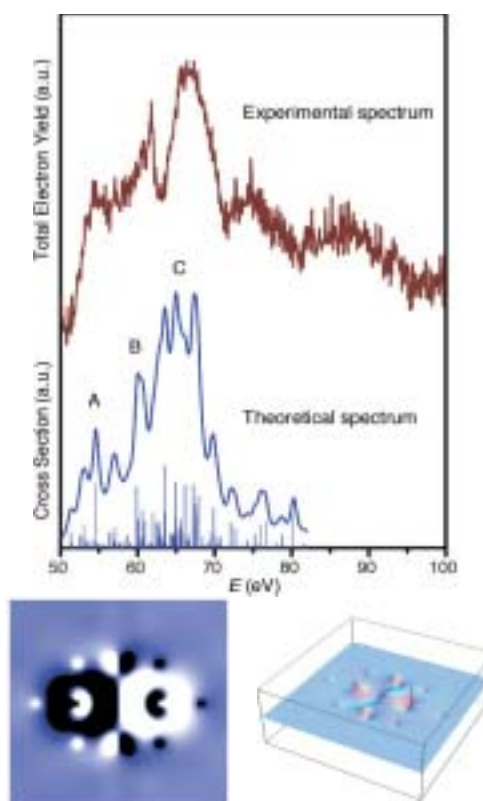


Figure 2. Li K absorption spectra of Li metal and wave functions for the exciton peak of LiF.

States and Structures

- Electron Microscopy and Crystal Chemistry -

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University of Leuven, Belgium, 10–11 January 2002
Max-Planck-Institute for Polymer Research, Germany, 1–2 February 2002
Max-Planck-Institute for Polymer Research, Germany, 2–20 December 2002

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 2002)

Presentations

Electrical properties of CuPcF_{16} films with top and bottom FET electrodes, Minari T *et al.*, 49th The Japan Society of Applied Physics., 27 March.

Development of a cold-FEG with a build-up tip for STEM, Kurata H *et al.*, Strategies and Advances in Atomic Level Spectroscopy and Analysis, 9 May.

Quantitative analysis of high resolution TEM images for CaF_2 and BaF_2 , Tsujimoto M, Takano H, Ogawa T *et al.*, 58th Annual Meeting Elec. Micro., 14 May.

Application of ELNES to local analysis, Kurata H, Hojou K(JAERI), 58th Annual Meeting Elec. Micro., 16 May.

Observation of formation process of metal nano-rod by cryo-TEM, Hayashi M, Ogawa T, Isoda S, 58th Annual Meeting Elec. Micro., 16 May.

High-resolution observation of the surface of M-Phc

crystals, Moriguchi S, 58th Annual Meeting Elec. Micro., 16 May.

Fast electron energy-loss spectroscopy on metal phthalocyanines, Koshino M, Kurata H, Isoda S; 2nd Intern. Conf. Porphyrines and Phthaoocyanines, 3 July.

Organization of copper-phthalocyanine molecules on a mono-molecular organic layer, Takajo D *et al.*, 2nd Intern. Conf. Porphyrines and Phthaoocyanines, 2 July.

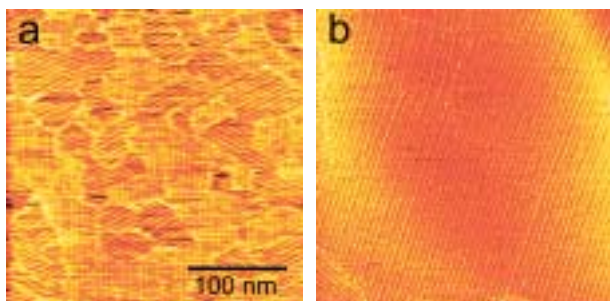
EELS analysis and DV- $X\alpha$ calculation for 7,7,8,8-tetracyanoquinodimethane (TCNQ) and tetrafluoro-TCNQ. Koshino M, Kurata H, Isoda S. 15th Annual Meeting Soc. DV- $X\alpha$ Japan, Jul. 31 - Aug. 2.

Expeimental estimation of dyanmical scattering effect on electron crystallography, Isoda S, Kuwamto K, Ogawa T, XIX Conference and General Assembly of the Intern. Union of Cryst., 8 August.

Monolayer and bilayer formation of 17, 19-dotetracontadiyne at a liquid/solid interface

Monolayer and bilayer of 17, 19-dotetracontadiyne (DTDY) on graphite substrate were studied by scanning tunneling microscopy at a liquid/solid interface of phenyloctane solution. The orientation of the layers was examined with respect to the HOPG. The first layer grew very quickly with many small domains with some tens nm in diameter, and the alkyl chains of the molecule in each domain align epitaxially along the a_g -axis of graphite (Fig.a). When the solution keeps at room temperature, the second layer of DTDY became to grow epitaxially on the first layer and the domain size was much larger than that of the first layer (Fig.b).

1. Takajo D, Fujiwara E, Irie S *et al.*, J. Cryst. Growth., **237-239**, 2071-2075 (2002).



Formation process of ultra fine platinum particles in an aqueous solution with surfactant

Formation process of ultrafine metal particles in water was examined with a cryogenic transmission electron microscope by using a rapid freezing specimen preparation technique. The particles were formed by hydrogen-reduction in an aqueous solution of chloroplatinic acid with or without a surfactant. The ultrafine platinum particle was obtained with the surfactant, and they were concluded to be formed not in a micelle as a nucleation site, but in arbitrary places in solution. During the formation process, the particles are coated and stabilized by surfactant molecules so as not to aggregate each other, when using the surfactant (Fig.c).

2. Hahakura S, Isoda S, Ogawa T *et al.*, J. Cryst. Growth., **237-239**, 1942-1945 (2002).

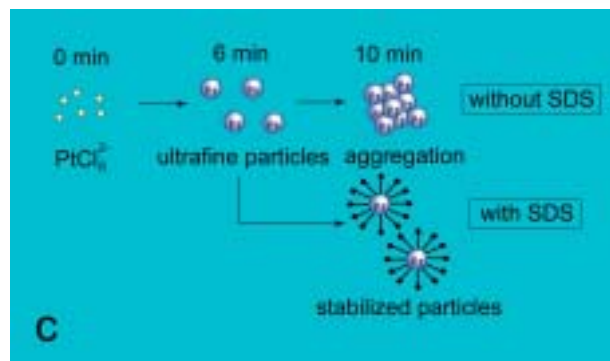
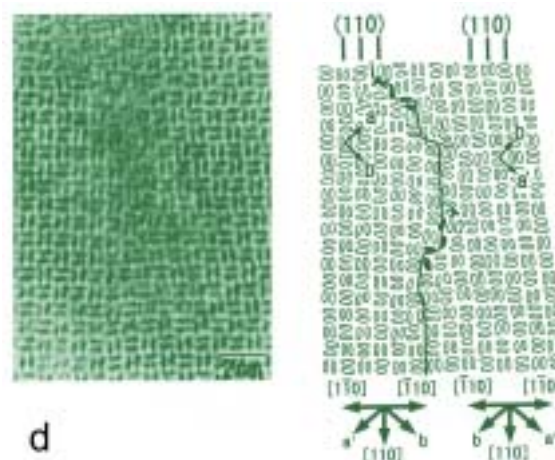
Two-dimensional crystal structures of the first and second layers of stearic acid at liquid/solid interface, Nemoto, T, Takajo D, Isoda S, XIX Congress of the Intern. Union of Cryst., 6 - 15 Aug.

Epitaxial growth and defect structure of quaterylene studied by high resolution electron microscopy

Vapor deposited epitaxial films of quaterylene on (001) of KCl were investigated using high-resolution electron microscopy and electron diffraction. The crystal c-axis is parallel and perpendicular to the substrate surface at a lower and at a higher temperature, respectively. This means that the long axis of the quaterylene molecule is in the film plane at a lower temperature and becomes perpendicular to it at a higher temperature.

High-resolution images revealed the detailed features of an edge dislocation, twin boundaries and small angle grain boundaries (Fig.d). Differing from the normal part of the crystal, the unit cells are deformed and the orientation of molecules are varied from unit cell to unit cell at defects. In addition, solitary molecular columns are seen to occupy empty spaces formed at the dislocation core or at the grain boundaries in order to relax the lattice distortion.

3. Maeda T, Isoda S, Kobayashi T, phys. stat. sol. (a)**191**, 489-498 (2002)



Grants

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 July 2002 - 31 March 2003.

States and Structures

- Polymer Condensed States -

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



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Visitors

Assoc Prof DI NOTO, Vito
Prof WHITE, James L
Prof RISEN Jr, William M

University of Padova, Padova, Italy, 8 February 2002
University of Akron, Akron, USA, 13 November 2002
Brown University, Providence, USA, 18 November 2002

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 2002)

Presentations

Structural analysis of the high-speed spun polyester fibers using the permanganic etching method, Yoshioka T, Tsuji M, Kawahara Y, et al., The 6th International Symposium organized by Inst. Chem. Res., Kyoto Univ. (ICRIS '02), January 31 - February 1 and other 4 presentations.

New insights into structural developments in natural rubber during uniaxial deformation by in-situ synchrotron X-Ray diffraction, Toki S, Murakami S, Kohjiya S, et al., Meeting of the Rubber Division, American Chemical Society, Savannah, Georgia, 29 April - 1 May.

Lamellar and crystalline-core thicknesses of the poly(3-oxotrimethylene) edge-on lamellae crystallized epitaxially from solution onto alkali halides, Tsuji M, Fujita M, Kohjiya S, Kawaguchi A, International Symposium on Polymer Crystallization, 9 - 12 June and other 2 presentation.

Biaxial tensile behaviors of elastomeric polymer net-

works, Kohjiya S, International Rubber Conference 2002, Prague, 3 July.

Volume phase transition of liquid crystalline gels, Urayama K, Okuno Y, Nakao T, et al., Polymer Networks 2002, France, 2 - 6 Sep, and related 6 presentations.

Conformational studies of an optically active 1,4-polyketone in solution and crystals, Kosaka N, Nozaki K, Tsuji M, et al., JSPS 51th Symposium on Macromolecules, 2 - 4 October, and other 3 presentations.

Devulcanization of unfilled natural rubber in supercritical carbon dioxide, Kojima M, Tosaka M, Kohjiya S, Ikeda Y, 162nd ACS Rubber Division Meeting, Pittsburgh, 8 - 11 October.

Structure of band-like cellulose assemblies produced by acetobacter xylinum, Hirai A, Tsuji M, Horii F, 1st International Cellulose Conference, 6 - 8 November.

Structural Development of Natural Rubber during Uniaxial Stretching

Structural development of natural rubber during uniaxial stretching was examined by an in situ wide angle X-ray diffraction (WAXD) measurement using a synchrotron and simultaneous stress-strain measurement. During stretching, the amorphous halo remained clearly even at 500% strain (Figure 1). That is, some polymer chains were oriented and crystallized, but considerable fraction of the chains were not oriented at all in spite of large deformations of the specimen. This result indicates that only minor fraction of polymer chains contribute to the stress and hysteresis loss during elongation.

1. Murakami S et al., *Polymer*, **43**, 2117 (2002).
2. Toki S et al., *Macromolecules*, **35**, 6578 (2002).

Volume Phase Transition of Liquid Crystalline Gels

We have firstly observed the volume phase transition of liquid crystalline (LC) gels accompanying the nematic-isotropic transition of LC molecules inside the gels[1]. The swelling of LC gels is mainly governed by nematic interaction, which is substantially different from the familiar swelling of isotropic gels mainly controlled by isotropic mixing interaction. Figure 2 displays the degree of equilibrium swelling as a function of temperature (T) for a LC gel in a low molar mass LC. Upon cooling, the isotropic swollen gel (a) is discontinuously transformed into the nematic shrunken gel (b) at T_{NI}^G . The nematic shrunken gel, surrounded by isotropic LC solvent, swells again in the region $T_{NI}^S < T < T_{NI}^G$. The nematic ordering of the surrounding solvent at T_{NI}^S yields an inflection in the swelling curve without discontinuity. A mean field theory successfully describes the complicated swelling and phase characteristics observed[2].

1. K. Urayama, Y. Okuno, T. Kawamura, S. Kohjiya, *Macromolecules*, **34**, 8252 (2001).
2. K. Urayama, Y. Okuno, T. Nakao, S. Kohjiya, *J. Chem. Phys.*, in press.

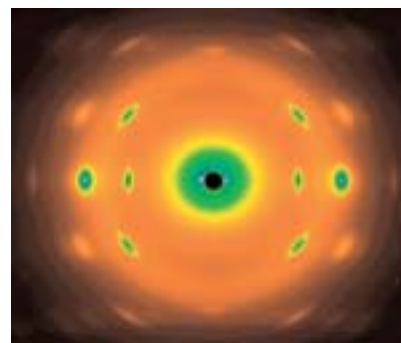


Figure 1. WAXD pattern of a natural rubber sample stretched up to 500% of the original length.

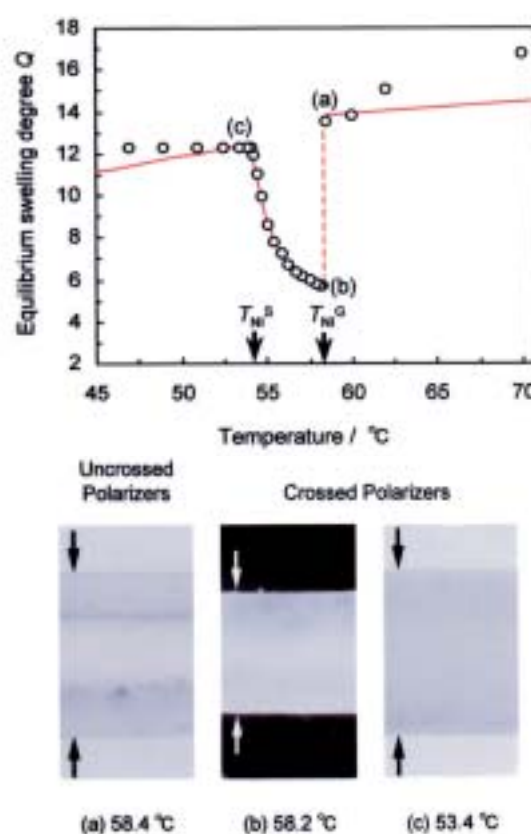


Figure 2. Equilibrium swelling - temperature curve of a nematic gel in a nematic solvent. The solid line represents the prediction of a mean field theory. The optical micrographs show the cylindrical gel in (a) totally isotropic phase; (b) nematic and isotropic phases inside and outside the gel, respectively; (c) totally nematic phase. The arrows indicate the boundary of the gel surface.

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, Direct observation of amorphous polymer network structures by TEM, Grant-in-Aid for Scientific Research, (B)(2), 1 April 2001 - 31 March 2003.

Urayama K, Dynamics of guest polymers in host poly-

mer networks, Grant-in-Aid for Scientific Research, Encouragement of Young Scientists, 1 April 2001 - 31 March 2003.

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

Interface Science

- Solutions and Interfaces -

<http://kaimen.kuicr.kyoto-u.ac.jp>



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MIKAWA, Kohei (M2)

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, crystallization of protein monolayers, and advanced dispersion systems are also investigated.

Research Activities (Year 2002)

Presentations

Water and Solutions under Extreme Conditions

Supercritical Water Decarboxylation of Aliphatic and Aromatic Carboxylic Acids, Nakahara M, 2002 International Association for the Properties of Water and Steam, 23 July.

NMR Study on Aqueous Solutions of Electrolytes at High Temperatures and High Pressures, Wakai C, Nakao N, Kubo M, Matubayasi N, and Nakahara M, 2002 International Association for the Properties of Water and Steam, 23 July.

Raman Spectroscopic Study of Supercritical Hydrogen Bonding Fluids, Kubo M, Matubayasi N, and Nakahara M, 25th Symposium on Solution Chemistry of Japan, 26 September.

Structure, Dynamics, and Reactions of Supercritical Water, Matubayasi N, 25th Symposium on Solution

Chemistry of Japan, 27 September.

Conformational Equilibria of Side Chains in Aspartic Acid Peptides and Achatin-I: Decomposition of the Thermodynamic Quantities, Sequence-Position Dependence, and Hydration Effect, Kimura T, Matubayasi N, and Nakahara M, 25th Symposium on Solution Chemistry of Japan, 27 September, and 26 related presentations in other meetings and symposia.

Ultra-thin Films

Effect of Infrared Radiation on FT-IR External Reflection Spectra of Langmuir Monolayers, Sakai H [Heian Jogakuin (Saint Agnes') College] and Umemura J, 55th Meeting of Colloid and Interface Chemistry, Japan, 14 September.

Dynamic NMR of Membrane-Drug Interactions

Solution NMR Studies on Distribution and Dynamics of Drugs in Membranes, Okamura E, 122th Annual Meet-

Raman spectroscopic studies of supercritical water and methanol: high-sensitivity observations over a wide density range

High-sensitivity Raman spectroscopic equipment is developed for the measurements of supercritical fluids. The system consists of a high-pressure chamber, a supercritical cell, a lens that collects back-scattered light, and a high-sensitivity Renishaw spectrometer connected to the collecting lens via fiber optic cable. The overview of the supercritical cell is shown in Fig.1. A specially manufactured thin diamond window enables an exceptionally wide solid angle observation so that the back-scattered light is collected by the detector with minimal loss. The new Raman cell system allows the vibrational analyses of supercritical water at 400°C and the density as low as $3.2 \times 10^{-4} \text{ g/cm}^3$ (corresponding to the pressure of 0.1 MPa). With the novel equipment, the density dependence of OH stretching bands of supercritical water and methanol were investigated over a wide range of densities. The OH symmetric stretching band of supercritical water shows a nonlinear density dependence at $\sim 0.2 \text{ g/cm}^3$ (corresponding to the reduced density of ~ 0.6) that was not observed in NMR chemical shift measurements. In contrast, the NMR chemical shift and the number of hydrogen bonds exhibit an excellent correlation with each other. The OH stretching band of supercritical methanol is generally related to the number of hydrogen bonds. From the fact that Raman spectroscopy and NMR chemical shift measurements show different density dependence, the number of hydrogen bonds cannot be a single representative indicator of the local structure.

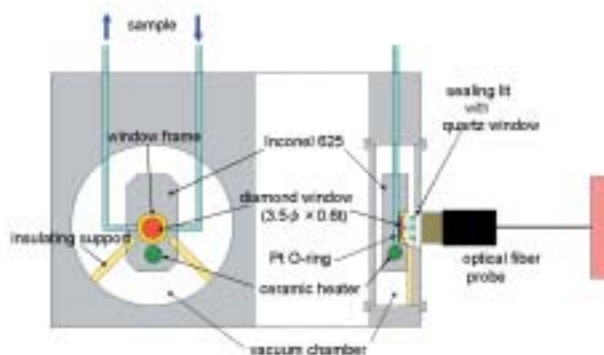


Fig. 1

Membrane dynamics and transport of endocrine disruptors and channel peptides

Membrane transport of endocrine disruptors (ED) and channel peptides is noninvasively detected by NMR. A high-resolution NMR combining pulsed-field-gradient technique shows how fast ED and peptides are transported in lipid bilayer vesicles, a good model for cell membrane. The transport of ED and channel peptides in membrane is not rapid but more than one order of magnitude as slow as that in solution. The transport is dominated by the membrane softness or fluctuation; the mobility is comparable to the membrane lipid diffusion. The success opens the possibility to monitor wide range of membrane transport phenomena; neither labeling nor probing is required.

ing of the Pharmaceutical Society of Japan, 26 March.

Static and Dynamic NMR Studies on Drugs and Endocrine Disruptors at Lipid Bilayer Interfaces, Nakahara M, NATO-ASI (EMLG/JMLG Annual Meeting): Novel Approaches to the Structure and Dynamics of Liquids, 12 September.

Dynamics of Lipid Bilayer Membranes and Drug Transport by NMR, Okamura E and Nakahara M, 55th Meeting of Colloid and Interface Chemistry, Japan, 14 September, and 2 related presentations in other 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, Element Organic Reactions in Super-

and Subcritical Water, Grant-in-Aid for Creative Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

Hasegawa T and Umemura J, Study of Molecular Recognition Formed in Systematic Molecular Assemblies, The Japan-USA Joint Research Projects, 1 April 2000 - 31 March 2003.

Matubayasi N, Theory of Solutions in the Energy Representation from Ambient to Supercritical, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

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



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YAMAGAMI, Takashi (M1)

Scope of Research

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

Research Activities (Year 2002)

Presentations

Studies on Solid State Chemistry of Organic Thin films Centering on Observation of Their Electronic Structures, Sato N, The 8th Organic Crystals Symposium (Tokyo, Japan), 27 March.

Electronic Structures of Unoccupied States in Lithium Phthalocyanine Thin Films of Different Polymorphs Studied by IPES, Sato N, Yoshida H, Tsutsumi K, Sumimoto M (Kumamoto U.), Fujimoto H (Kumamoto U.), Sakaki S (Dept. Mol. Eng.), The 11th International Conference on Solid Films and Surfaces (Marseille, France), 8 - 12 June.

Dielectric Imaging of Biological Cells and Tissues by a Scanning Probe, Asami K, 2nd International Conference on Broadband Dielectric Spectroscopy and its Applications (Leipzig, Germany), 2 - 6 September.

Insulator-Conductor Transition in a Hydrated Crystal of Squaric Acid Induced by a High Electric Field, Kita Y,

Terao H (U. Tokyo), Sugawara T (U. Tokyo), Sato N, The 2nd International Conference on Broadband Dielectric Spectroscopy and its Applications (Leipzig, Germany), 2 - 6 September.

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.

Tsutsumi K, Inverse Photoemission Spectroscopic Study on Contribution of Free Electron Nature to the Electronic Structure of Unoccupied States in Long Chain Alkanes, Grant-in-Aid for JSPS Fellows, 1 April 2002 - 31 March 2003.

Unoccupied electronic states in a hexatriacontane thin film studied by inverse photoemission spectroscopy

The electronic structure of low-lying unoccupied electronic states in a hexatriacontane ($n\text{-C}_{36}\text{H}_{74}$, HT) thin film was measured using inverse photoemission spectroscopy (IPES). While IPES permits direct observation of the unoccupied DOS, it is essential to avoid radiation damage and/or surface charging for the measurements of organic samples in particular. In this work it was practically confirmed that the HT thin film is easily degraded by electron irradiation. In order to check these influences we measured IPE spectra with different current densities of incident electrons, and by reducing the current density gradually we finally obtained a reliable IPE spectrum free from radiation effects at the current density bringing about our signal detection limit as shown in Fig. 1(a).

As a result, we have concluded that the only IPE spectrum of HT reported previously by Dudde and Reihl was significantly influenced by the electron bombardment. The observed spectrum shows two distinct features near the vacuum level: they were not resolved in the reported spectrum. The reliable information of DOS for the lowest unoccupied states in HT seems to be first obtained here.

The two features correspond to those so far estimated from other electron spectroscopies, while uncertainty remains in the absolute energy of the IPE spectrum. Our spectrum is further compared with the reported results of theoretical calculations concerning the unoccupied electronic states in long chain alkanes. As a result, we have tentatively assigned the first and the second spectral features to $1b_{1u}$ and $2b_{3u}$ states, respectively, by comparing the intensity ratio for those features with that in the DOS estimated from the reported extended Hückel calculation.



Prof. Dr. Frank Willig from Hahn-Meitner-Institute, Berlin, Germany, gave a stimulating seminar.

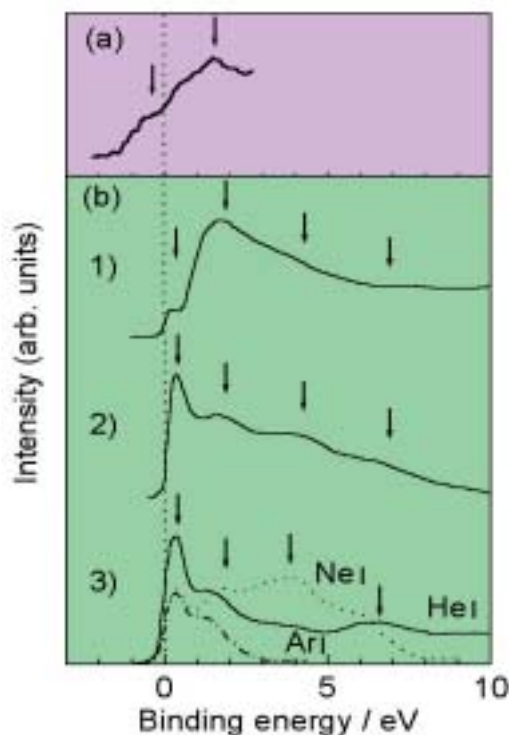


Fig. 1. The most reliable IPE spectrum of an HT thin film (a) obtained at the electron current density of $3.4 \times 10^{-4} \text{ A m}^{-2}$, compared with the spectra regarding the lower unoccupied states of HT thin films obtained by the different electron spectroscopic methods: (b) 1) LEETS, 2) SEES and 3) UPS. Arrows indicate distinct spectral features. UP spectra were measured with different excitation energies indicated beside the respective spectra.

Dielectric imaging of biological cells and tissues using a scanning probe technique

For characterizing structural and electrical properties of biological cells and tissues, a dielectric imaging technique using a scanning fine probe is available. Since dielectric images of cells and tissues are closely related to their morphology, it is important to compare the dielectric images with optical ones directly. In this study, therefore, a scanning dielectric probe unit was assembled on an inverted optical microscope. The scanning probe unit consisted of an X-Y stage controlled by a computer, a fine coaxial probe and a chamber for samples that had an ITO glass electrode at the bottom. Dielectric measurement was made by the three-terminal method that can restrict the measurement to a small area because of eliminating fringing fields. The performance of the system was tested with well-defined nylon and stainless steel meshes in water, and also with epithelia of plant leaves in water, the lateral resolution being around 10 nm using a probe with a Pt wire of 25 nm in diameter.

Interface Science

- Hydrospheric Environment Analysis -

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



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Assoc Prof Tomasz T.
Prof Rudolf Durny

Polish Academy of Science, Poland, 1 November, 2001
Slovak Technical University, Slovakia, 8–15 March, 2002

Scope of Research

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

Research Activities (Year 2002)

Presentations

Solvent Extraction of Metal Ions with Novel 4-Acyl-5-pyrazolones Having Crown Ether Moiety as Intramolecular Synergist, Umetani S, Yamazaki S (Nara U. Educ.), Ogura K (Ube Nat. C. Tech.), International Solvent Extraction Conference (ISEC 2002), 20 March.

$^{240}\text{Pu}/^{239}\text{Pu}$ isotopic ratio in the western northwest Pacific Ocean, Norisuye K, Okamura K, Sohrin Y, et al., Goldschmidt Conference 2002, 19 August.

Tungsten and molybdenum in hydrothermal fluids of the Izu-Bonin Arc and the Okinawa Trough, Sohrin Y, Kishida K, Okamura K, et al., Goldschmidt Conference 2002, 22 August.

Bioactive trace metals in the North Pacific Ocean, Sohrin Y, SCOR-JOS International Symposium, 1 October.

Development of a deep-sea in-situ chemical analyzer and its application for hydrothermal field observation, Okamura K, SCOR-JOS International Symposium, 1 October.

Behaviors of Mn and Fe in hydrothermal plumes and diffused flows at the Suiyo Seamount, Izu-Bonin arc, Okamura K, Suzuki M, Sohrin Y, et al, AGU 2002 Fall Meeting, 8 December.

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.

Umetani S, Design of highly selective recognition and separation system of metal ions, Grant-in-Aid for Scientific Research (C) (1), 1 April 2001 - 31 March 2003.

Okamura K, Development of *in situ* measurement system of CO_2 related matter in seawater for global warming control, NEDO Grant, 1 April 2001 - 31 March 2004.

Awards

Kitano T, The ICR Award for Students.

Tungsten is a unique probe into the evolution of submarine hydrothermal fluids

Submarine hydrothermal activities play an important role in the circulation of elements on the earth and the formation of orebody. However, many trace elements in hydrothermal fluids have not been determined yet, due to difficulties in sampling and analysis. Here we report the first concentrations of W in hydrothermal fluids. The concentrations of W in endmember fluids (0.21-123 nmol/kg) reach 4 orders of magnitude above ambient levels in seawater, suggesting that the hydrothermal activities are a critical source of W to the ocean. Since W is a unique chemical species in showing a large variation depending on a hydrothermal site and being not incorporated into silicate and sulphide mineral phases, W can be a probe to elucidate the evolution conditions of hydrothermal fluids. We also show that Mo decreases in hydrothermal fluids to one hundredth of seawater due to precipitation of Mo sulfide. These results suggest that a W/Mo ratio can be a proxy in paleoceanography. It should have been increased in seawater when an oceanic anoxic event occurred or when the hydrothermal activity was more vigorous.

$^{240}\text{Pu}/^{239}\text{Pu}$ isotopic ratio in the western north-west Pacific Ocean

Plutonium is one of the long-lived anthropogenic radioelements and is a useful chemical tracer in the ocean. It has been introduced into the ocean via stratospheric fallout from nuclear tests that peaked in 1962, but it is suggested that plutonium in the Pacific Ocean has also been derived from close-in tropospheric fallout. Isotopic analysis using high sensitive mass spectrometry is a powerful tool to specify these origins in the ocean. However, few studies for plutonium isotopic analysis have been made. Here we report $^{240}\text{Pu}/^{239}\text{Pu}$ isotopic ratio in the western northwest Pacific Ocean.

Large volumes of seawater samples (800~4,200 l) were collected from the Sea of Japan, Okhotsk Sea, and north-west Pacific during the KH98-3 cruise of R/V Hakuho-Maru in July-August, 1998. Plutonium was extracted from seawater using MnO_2 -impregnated fibers and separated from uranium by solvent extraction. $^{240}\text{Pu}/^{239}\text{Pu}$ isotopic ratio in the final sample solution was determined by ICP-MS.

The isotopic ratios at CM6 (45°25'N 145°05'E), CM12 (41°21'N 137°20'E), CM20 (37°44'N 135°14'E) and CM22 (40°00'N 145°00'E) were found to be in the range of 0.20-0.23, which were not so different from the average global fallout ratio of 0.18. However, these isotopic ratios and

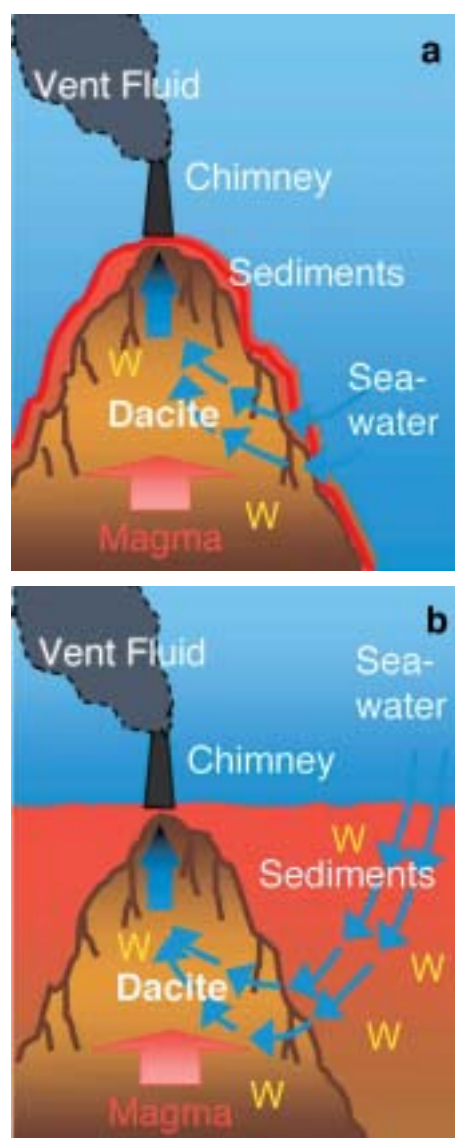


Fig. Schematic diagrams of W enrichment mechanism in hydrothermal fluids at the arc-backarc settings. (a) a sediments-starved vent of the Suiyo Seamount. (b) a sediments-rich vent of the Okinawa Trough. At the both vents, water-rock (dacite) interaction at high temperature (~400°C) is a source of W. Reaction with terrigenous sediments at low temperature (~100°C) is another important source of W at the Okinawa Trough.

previously measured $^{240}\text{Pu}/^{239}\text{Pu}$ ratios in the North Pacific except for locally contaminated regions, seem to be slightly higher than the global fallout ratio, suggesting possibility of plutonium from close-in tropospheric fallout in 1950s. The precise measurement of $^{240}\text{Pu}/^{239}\text{Pu}$ isotopic ratio by multi-collector (MC) ICP-MS and determination of ^{238}Pu and ^{241}Pu activity by alpha spectrometry are the further works to clarify the matter.

Solid State Chemistry - Artificial Lattice Alloys -

<http://ssc1.kuicr.kyoto-u.ac.jp>



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Visitor

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Institute of Physics, Polish Academy of Sciences, Poland, 9 February–8 May 2002

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 2002)

Presentations

Magnetization Switching of the Vortex Core at the Center of Circular Permalloy Dot, Okuno T, Shigeto K, Mibu K, Shinjo T, Yokoyama Y (AIST), Suzuki Y (AIST), Ono T (Osaka Univ.), 17th International Colloquium on Magnetic Films and Surfaces, 5 March.

Magnetic Domain Wall in a Nano-Contact between Two NiFe Wires, Miyake K, Shigeto K, Mibu K, Shinjo T, Suzuki Y (AIST), Yokoyama Y (AIST), Ono T (Osaka Univ.), 17th International Colloquium on Magnetic Films and Surfaces, 7 March.

Growth-Orientation Dependence of Cr Magnetic Moments in Fe/Cr Multilayers Studied using ^{119}Sn Mössbauer Spectroscopy, Jiko N, Almokhtar M, Mibu K, Shinjo T, 57th Annual Meeting of the Physical Society of Japan, 25 March.

The Variation of the Magnetic Structure of the Domain Wall Formed in the Nano-Contact between Two NiFe Wires, Miyake K, Shigeto K, Mibu K, Shinjo T, Yokoyama Y (AIST), Suzuki Y (AIST), Ono T (Osaka Univ.), 57th Annual Meeting of the Physical Society of Japan, 25 March.

Size Dependence of Switching Field of Turned-Up Magnetization at the Center of a Magnetic Dot, Okuno T, Shigeto K, Ono T (Osaka Univ.), Yokoyama Y (AIST), Suzuki Y (AIST), Mibu K, Shinjo T, 57th Annual Meeting of the Physical Society of Japan, 25 March.

Switching of Turned-Up Magnetizations in a Cross-

Tie Wall in a Magnetic Dot, Okuno T, Shigeto K, Ono T (Osaka Univ.), Mibu K, Shinjo T, 2002 Autumn Meeting of the Physical Society of Japan, 6 September.

Magnetism of Cr in Cr(110)/Sn Multilayers, Jiko N, Mibu K, Takeda M (Tohoku Univ.), Suzuki J (JAERI), Shinjo T, 2002 Autumn Meeting of the Physical Society of Japan, 8 September.

Curie Temperature and Magnetic Properties of Gd Layers in Gd/Cu Multilayers, Ohkochi T, Hosoi N, Mibu K, 2002 Autumn Meeting of the Physical Society of Japan, 8 September.

The Observation of a Magnetic Domain Wall Injected into a Ferromagnetic Wire, Miyake K, Mibu K, Shinjo T, 2002 Autumn Meeting of the Physical Society of Japan, 8 September.

Magnetic Structure of a Diamond Shape Dot Array Connected with Nano-Contacts, Miyake K, Mibu K, Shinjo T, 26th Annual Conference on Magnetism in Japan, 17 September.

Award

Poster Award, Magnetic Domain Wall in a Nano-Contact between Two NiFe Wires, Miyake K, *et al.*, 17th International Colloquium on Magnetic Films and Surfaces, 7 March.

Magnetic Structures of Diamond-Shaped NiFe Dot Arrays

Arrays of diamond-shaped NiFe dots were fabricated by an electron-beam lithography and lift-off method, and the magnetization arrangements were investigated using magnetic force microscopy. Typical size parameters and a scanning electron microscopy image are shown in Fig 1. The thickness of the sample was set to be 10 nm. A series of patterns with different designed distance between dots were drawn by electron beams on the same substrate. It was found that disconnected dot arrays and connected dot arrays with different contact sizes were incidentally fabricated after the lift-off process.

Figure 2 shows a magnetic force microscopy image at zero field after a magnetic field of 5 kOe was applied parallel to the short axis of the dots. The magnetic charge distribution appears as black and white contrasts. It is clearly shown that each dot has a single magnetic domain state and the magnetization aligns along the long axis of the dots. The magnetizations in neighboring dots are oriented antiparallel with a few exceptions due to magneto-static interaction between the dots. Eventually, a very small domain wall is effectively confined in each nano-contact area. Such samples are promising model systems to investigate magnetoresistance caused by magnetic domain walls.

Magnetization Reversal of Turned-Up Magnetization in Track-Shaped NiFe Dots

When a circular dot is fabricated from a soft magnetic material such as NiFe, a magnetic vortex structure is stabilized due to a competition between exchange interaction and magnetostatic interaction. A nanoscale singularity spot with perpendicular magnetization, which is called "turned-up magnetization", is formed at the center of the vortex. Such a singularity spot appears not only at the center of a "circular-vortex", but also at the center of an "anti-vortex". In order to investigate magnetization reversal of turned-up magnetizations at both types of vortex cores, track shaped (quasi-ellipsoidal) submicron dots with 50 nm in thickness were made of NiFe alloy using electron-beam lithography (Fig. 3). The switching field of turned-up magnetization for magnetic field normal to the sample plane was measured using magnetic force microscopy. It was found that the switching field at the anti-vortex core is smaller than that at a circular-vortex core by about 1000 Oe. It was also demonstrated that the direction of the magnetizations at three singularity spot can be controlled by applying magnetic field perpendicular and parallel to the sample plane.

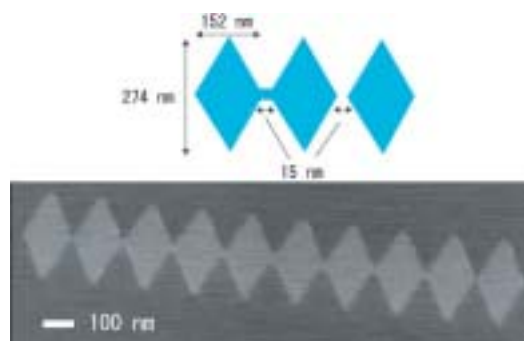


Fig. 1 Illustration of the sample structure and scanning electron microscopy image of diamond-shaped NiFe dot arrays.

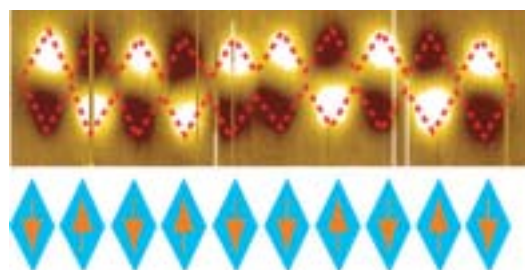


Fig. 2 Magnetic force microscopy image and schematic illustration of the magnetic structure. The red dashed lines indicate the shape of the dots.

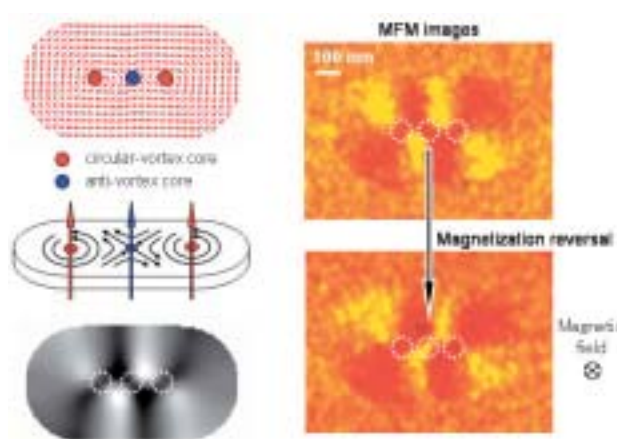


Fig. 3 Circular-vortex cores and an anti-vortex core formed in a track-shaped NiFe dot, and magnetization reversal of turned-up magnetization at the anti-vortex core.

Solid State Chemistry - Quantum Spin Fluids -

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Scope of Research

Quantum spin oxide systems such as high- T_c superconducting cuprates, $\text{La}_{2-x}(\text{Ba,Sr})_x\text{CuO}_4$, $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ and $\text{Pr}_{2-x}\text{La}_x\text{Ce}_x\text{CuO}_4$ are synthesized in the form of single crystals using traveling-solvent-floating-zone method. Detailed equilibrium phase diagram of Pr_6O_{11} - La_2O_3 - CuO system is also investigated to elucidate the effect of oxygen nonstoichiometry on these oxide. Main subjects and techniques are: mechanism of high- T_c superconductivity: origin of quantum phase separation in strongly correlated electron systems: spin excitations in quantum spin systems: interplay between spin and charge flow in doped spin system: neutron scattering by using triple-axis as well as time-of flight techniques.

Research Activities (Year 2002)

Presentations

A comparative study on the magnetic order in hole- and electron-doped cuprates, K. Yamada, M. Fujita, T. Uefuji, H. Goka, M. Matsuda, I. Watanabe, K. Nagamine, The 23th International Conference on Low Temperature Physics, Hiroshima, Japan, 26 Aug. 2002.

Magnetic excitation in the spin-glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, H. Goka, S. Kuroshima, M. Fujita, K. Yamada, The 23th International Conference on Low Temperature Physics, Hiroshima, Japan, 26 Aug. 2002.

Doping effect on magnetic order and superconductivity in electron-doped cuprate single crystals $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$, T. Uefuji, T. Kubo, S. Kuroshima, M. Fujita, K. Yamada, M. Matsuda, I. Watanabe, K. Nagamine, CREST International Workshop on Novel Quantum Phenomena in Transition Metal Compound, Sendai, Japan, 30 Aug. 2002.

Phases and their relations in the Pr_6O_{11} - La_2O_3 - CuO system, Y. Ikeda, K. Yamada, Y. Kusano, J. Takada, 10th International Ceramic Congress & 3rd Forum on New Materials, Florence, Italy, 16 July 2002.

Spin dynamics of pure and diluted $S=1/2$ Kagome-like magnetic system $(\text{Cu}_x\text{Zn}_{1-x})_3\text{V}_2\text{O}_7(\text{OH})_2\text{H}_2\text{O}$, A. Fukaya, Y. Fudamoto, I.M. Gat, T. Ito, M. Larkin, A.T. Savici, Y.J.

Uemura, P.P. Kyriaku, G.M. Luke, M.T. Rovers, K.M. Kojima, A. Keren, M. Hanawa, Z. Hiroi, 9th International Conference on Muon spin rotation/relaxation/resonance, Williamsburg, VA, USA, 4 Jun. 2002.

Grants

Yamada K, Study of quantum phase separation in the transition metal oxides, Grant-in-Aid for Scientific Research on Priority Areas (Novel Quantum Phenomena in Transition Metal Oxides), 1 April 2000 - 31 March 2003.

Yamada K, Study of X-ray inelastic scattering study on the charge and lattice dynamics in metal oxides, Grant-in-Aid for Scientific Research (B), 1 April 2002 - 31 March 2004.

Fujita M, Study of High- T_c superconductivity mechanism in the electron-doped cuprates, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2001 - 31 March 2003.

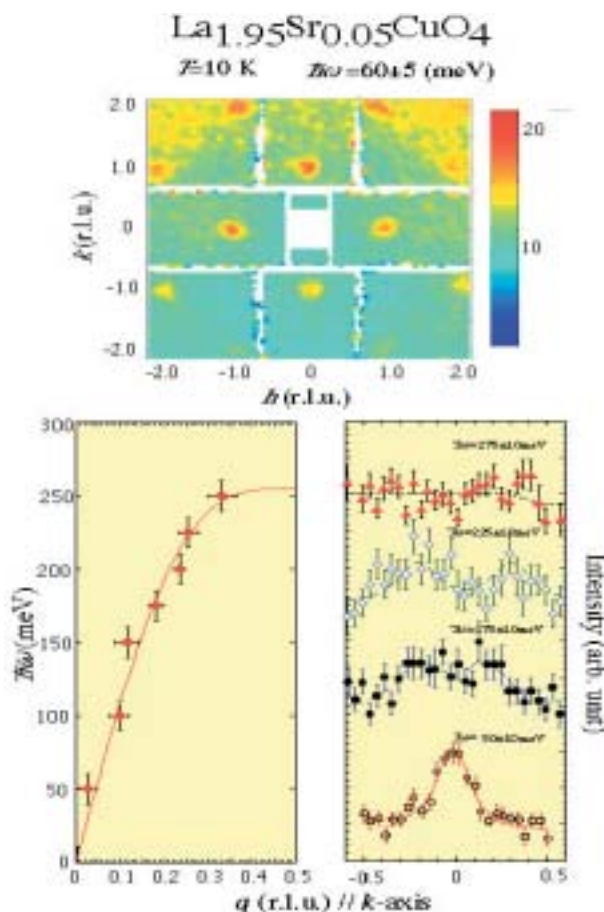
Yamada K, Collaboratory on Electron Correlations-Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2001 - 31 March 2006.

Magnetic excitation in spin-glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

Magnetic excitation in the spin glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ($x=0.05$) which is located near the lower critical concentration of high- T_c superconductivity was observed up to 300 meV by pulsed neutron scattering experiment. The upper figure is a contour map showing the square lattice of inelastic magnetic peaks at $\omega=60$ meV and $T=10$ K.

In the energy region below ~ 50 meV, the magnetic peak width decreases with increasing energy. On the other hand, over ~ 50 meV, it increases with energy, and we can draw a similar dispersion curve as observed in La_2CuO_4 (lower figure). The nearest neighbor interaction J was evaluated to be 108 ± 6 meV which is slightly smaller than that of La_2CuO_4 by applying the 2D antiferromagnetic dispersion relation.

The imaginary part of dynamical magnetic susceptibility $\chi''(\omega)$ decreases monotonically up to ~ 50 meV with energy and become almost energy-independent in the energy region of >50 meV like La_2CuO_4 . The above-mentioned features indicate that it is possible that the spin fluctuation in the low energy region (<50 meV) crosses over to that of spin wave-like.



Upper panel: A contour map of intensity of scattered neutron. Spots making square lattice are magnetic excitations. Lower panel: The energy dependence of magnetic excitation (right) and the dispersion deviated from these data (left).

Reversible precipitation and resolution phenomenon in $\text{Pr}_{2-x}\text{La}_x\text{CuO}_4$ ($1.35 < x < 1.5$)

Solid-solubility range and phase stability of $\text{Pr}_{2-x}\text{La}_x\text{CuO}_4$ ($0 < x < 2$) have been studied mainly from high temperature X-ray diffraction, thermogravimetric analysis (TGA), differential thermal analysis (DTA), and TEM observation. There are two tetragonal T' -type solid solutions with slightly different lattice constants in Pr_2CuO_4 - La_2CuO_4 system. We observed an interesting phenomenon in $\text{Pr}_{2-x}\text{La}_x\text{CuO}_4$ ($1.35 < x < 1.5$) (T'_B) as shown schematically in Fig. 1. High temperature X-ray diffraction measurement of T'_B phase reveals phase segregation into three phases (T'_B -, T -type, and unknown phase) upon heating process at around 900°C in O_2 . Surprisingly, in the cooling process, reformation into original T'_B phase occurred at around 200°C. At the same time, a sintered pellet transforms into fine powder ($\sim 10 \mu\text{m}$) in a few ten seconds. This reaction occurred completely reversible upon cyclic heat treatment. Reversibility of the phenomenon was also confirmed by TGA and DTA measurement. To our best of knowledge, these phenomena have not been reported in high- T_c superconductor related cuprates.

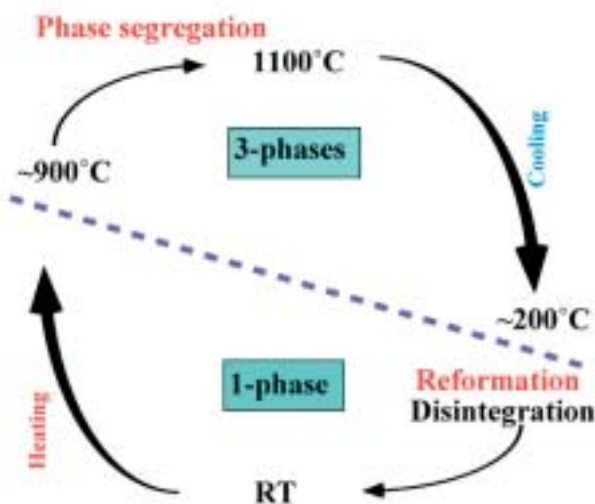


Figure 1. A schematic representation of a reversible phase change for T'_B phase.

Solid State Chemistry

- Solid State Chemistry -

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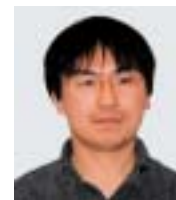
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Prof RAO, C. N. R. Jawaharlal Nehru Centre for Advanced Scientific Research, India, 11 March 2002

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 2002)

Presentations

Single Crystal Growth of Perovskites and Related Compounds at Several GPa, Azuma M, Saito T, Ishiwata S, Yamada I, Takano M, MRS 2002 Spring Meeting, 1-5 April.

Formation of Two Novel Zirconium Phosphates Controlled by Organic Solvents, Yu R, Wang D, Kumada N, Kinomura N, Matsumura Y, Takano M, Fifth International Conference on Solvothermal Reactions (ICSTR), 22 - 26 July.

Hydrothermal Formation of Novel Cerium Materials with Open-Framework Architectures, Yu R, Wang D, Takei T, Kumada N, Kinomura N, Takano M, International

Symposium on solid State Chemistry in China, 9 - 12 August.

Single Crystal Growth of $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}$ and Related Compounds at High Pressure of Several GPa, Azuma M, Saito T, Ishiwata S, Yamada I, Takano M, Kohsaka Y, Takagi H, 2002 International Conference on Physics and Chemistry of Molecular and Oxide Superconductors, 13 - 18 August.

Iron Oxides Revisited: Solid State Chemistry, Takano M, The 2nd Hiroshima Workshop-Transport and Thermal Properties of Advanced Materials, 16 - 19 August.

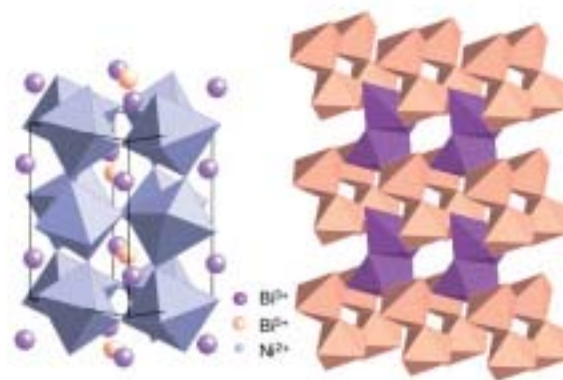
Single crystal growth of transition metal oxides at high pressures of several GPa

High pressure synthesis is a powerful technique to search for new materials. Generally speaking, however, it used to be almost impossible to obtain single crystal samples of these high-pressure phases. We have developed a technique to grow single crystals of transition metal oxides by means of flux methods based on the synchrotron X-ray powder diffraction studies at high pressures of several GPa. Magnetic, electrical and optical measurements on the grown crystals are being performed.



Crystal structure and physical properties of new Ni(II) perovskite BiNiO_3

New triclinic perovskite BiNiO_3 has been synthesized at a high pressure of 6 GPa with high oxidizing atmosphere. Structure refinement based on synchrotron X-ray powder diffraction and bond valence calculation revealed the disproportionation of Bi ions into Bi^{3+} and Bi^{5+} . Both of these were coordinated in distorted BiO_6 octahedra reflecting the strong covalency of Bi-O bonds. Because of the presence of the highly oxidized Bi^{5+} , the oxidation state of Ni was 2+ and BiNiO_3 thus showed insulating behavior with localized $S=1$ magnetic moments.



Single Crystal Growth of Transition Metal Oxides at High Pressures of Several GPa, Azuma M, Saito S, Niitaka S, Ishiwata S, Kanda H, Yamada I, Kohsaka Y, Takagi H, Takano M, 15th International Symposium on Superconductivity (ISS2002), 11 - 13 November.

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_3 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, Physical properties of oxychloride superconductor crystals grown at high pressures. Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

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

Awards

Azuma M, JSPM Award for Innovative Research.

Search for new transition metal oxides and single crystal growth by means of high pressure synthesis.

The Japan Society of Powder and Powder Metallurgy.

Solid State Chemistry - Amorphous Materials -

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



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Dr M Singh NASA Glen Research Center, USA, 24 May, 2002

Scope of Research

In this laboratory, amorphous and polycrystalline inorganic materials with various optical functions such as photorefractivity, optical nonlinearity, and photo-catalysis are the target materials, which in the forms of thin film and bulk are synthesized mainly by the sol-gel, multi-cathode sputtering, melt-quenching and sintering methods. In order to obtain highly functional materials the detailed structure is extensively investigated by using X-ray diffraction techniques, high-resolution NMR, thermal analyses, various laser spectroscopies and ab initio molecular orbital calculations, and so on.

Research Activities (Year 2002)

Presentations

Preparation and optical properties of organic/inorganic hybrid low-melting glasses, Masai H, Takahashi M, Yoko T, India-Japan Information Technology Discussion-Meeting, 15 March, Spring meeting Ceramic Soc. Jpn., 26 March, XIIIth International symposium on non-oxide glasses and new optical glasses, 12 September, Meeting on Glass and Photonics Materials, 22 November.

Photocatalysis of TiO_2 thin film electrodes, Mori R, Takahashi M, Yoko T, Spring meeting Ceramic Soc. Jpn., 23 March, Autumn meeting Chem. Soc. Jpn., 25 September.

Photosensitive GeO_2 - SiO_2 films for UV laser writing of waveguides, Sakoh A, Takahashi M, Nishii J (AIST), Yoko T, Spring meeting Jpn. Soc. Appl. Phys., 29 March, Laser Precision Microfabrication, 27 May, Glass and op-

tical materials division fall meeting, ACerS, 15 September, Meeting on Glass and Photonics Materials, 21 November.

Structural analysis of glasses using high-resolution NMR and ab initio molecular orbital calculation method, Tokuda Y, Miyabe D, Mizuno M, Yoko T, Glass and optical materials division fall meeting, ACerS, 15 September, Meeting on Glass and Photonics Materials, 22 November.

Optical properties of dielectric multilayer structures with the dual-periodicity, Akita Y, Shimada R, Takahashi M, Yoko T, Fall meeting Ceramic Soc. Jpn., 22 September, International workshop on PECS4, 29 and 30 October.

Waveguide formation in niobium tellurite glasses, Tokuda Y, Saito M, Takahashi M, Yoko T, XIIIth International symposium on non-oxide glasses and new optical glasses, 12 September.

Preparation of organic/inorganic hybrid low-melting glasses

Organic/inorganic hybrid low-melting glasses free of pollution elements such as Pb and F, the use of which has been omitted from the viewpoint of environmental protection, are developed by using sol-gel melting and non-aqueous acid-base reaction processes. This new type of glass can contain a large amount of optically functional organic materials, which have high non-linear susceptibility at the optical communication wavelength (1.3~1.5 μm). A number of organic materials are examined to establish the optimum performance in these hybrid glasses. One example of such functional organic materials is fullerene (C_{60}), which has been successfully introduced into the present hybrid low-melting glass. The use of these materials renders the glass very suitable for many applications in photonic devices.



C_{60} -doped low-melting glass

Photosensitive GeO_2 - SiO_2 films for UV laser direct writing of waveguides

Recent results have suggested that p-CVD-deposited silica glass films doped with large amounts of GeO_2 exhibit a significant photorefractivity. In fact direct writing of channel waveguide structures in the p-CVD GeO_2 - SiO_2 glass films have been successfully carried out implementing UV laser irradiation. A propagation of light with wavelengths of 488 nm and 1553 nm were experimentally confirmed with this channel waveguides.

Optical properties of dielectric multilayer structures with dual-periodicity

Dielectric multilayer structures with dual-periodicity have been found to exhibit several interesting features. Among them, a strong localized state of Bloch photons in a particular condition is expected to enhance the electromagnetic field. The dual-periodic multilayer structures consisting of SiO_2 and TiO_2 films, which are attained by modulating the thickness of TiO_2 layers with a high dielectric constant, was deposited on a silica glass substrate by helicon plasma sputtering. The transmission properties of these structures with different modulation parameters and their thermal response in the temperature region from RT to 200°C are examined aiming at the possible applications as an active switch.



The dual-periodic multilayer structures with various thickness-modulation parameters. These layers are clearly uniform and the colours are somewhat beautiful.



Y-branch channel waveguide directly written by UV laser irradiation. Ar^+ laser light (488nm) is coupled.

Grants

Yoko T, Photochemical reactivity of glasses, Grant-in-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 active optical integrated circuit based on oxide glasses, Industrial Technology Research Grant Program, NEDO, 1 November 1999 - 31 March 2003.

Tokuda Y, Structure and optical nonlinearity of chalcogen-containing glasses, Grant-in-Aid for Scientific Research, Promotive research, 1 April 1999 - 31 March 2003.

Takahashi M, Development of photorefractive low-melt-

ing hybrid glasses, Asahi Glass foundation, 1 April 2000 - 31 March 2002.

Takahashi M, Preparation of novel low-melting glasses through non-aqueous acid-base reaction, Izumi Scientific foundation, 1 October 2001 - 31 September 2002.

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.

Shimada R, Study on optical devices using novel organic/inorganic hybrid low-melting glasses, Strategic Information and Communications R&D Promotion Scheme, Ministry of Public Management, Home Affairs, Posts and Telecommunications, 1 December 2002 - 31 March 2005.

Fundamental Material Properties - Molecular Rheology -

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Dr Steve Granick

University of Illinois, USA, 2 December 2002

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 2002)

Presentations

Rheo-Dielectric Behavior of Entangled Chains: An Approach to Convective Constraint Release, H. Watanabe, UCSB ITP Workshop for Dynamics of Complex and Macromolecular Fluids, 23 April.

Coarse Grained Dynamics Investigated by Dielectric and Viscoelastic Relaxation, H. Watanabe, Nagoya University International Workshop on Coarse-Grained Dynamics in Soft-Materials, 28 June.

Rheo-Dielectrics in Oligomeric and Polymeric Fluids, H. Watanabe, Pisa University III Workshop on Non-Equilibrium Phenomena in Supercooled Fluids, Glasses, and Amorphous Materials, 24 September.

Birefringence and Viscoelasticity of Polymers around the Glass Transition Zone, T. Inoue, Pisa University III Workshop on Non-Equilibrium Phenomena in Supercooled Fluids, Glasses, and Amorphous Materials, 24 September.

Rheology of Poly(Methyl Methacrylate-co-Styrene) Particles Suspended in Water: Electrostatic Interaction and Brownian Motion, H. Watanabe, Y. Matsumiya, T. Kanaya, Y. Takahashi, M. Horigome, M. Yada, and A. Miyakawa,

Japan-Korea-Australia Three Nation Conference on Suspension Rheology, 14 October.

Significance of the Longest Rouse Relaxation Time in the Stress Relaxation Process of Entangled Polymer Solutions, T. Inoue, and K. Osaki, Polymer Conference on the Mission and Challenges of Polymer Science and Technology, 4 December.

Grants

Watanabe H, Molecular rheology of amorphous polymer studied by electric birefringence, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

Inoue T, Molecular rheology of polymer solids, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

Matsumiya Y, Effect of branching and molecular weight distributions on entanglement relaxation, Grant-in-Aid for Scientific Research, 1 April 2001 - 31 March 2003.

Paul KRA, Development of a Model for Entanglement Dynamics of Polymers Having Multiple Coarse-graining Scales, Grant-in-Aid for Scientific Research, 1 April 2002 - 31 March 2004.

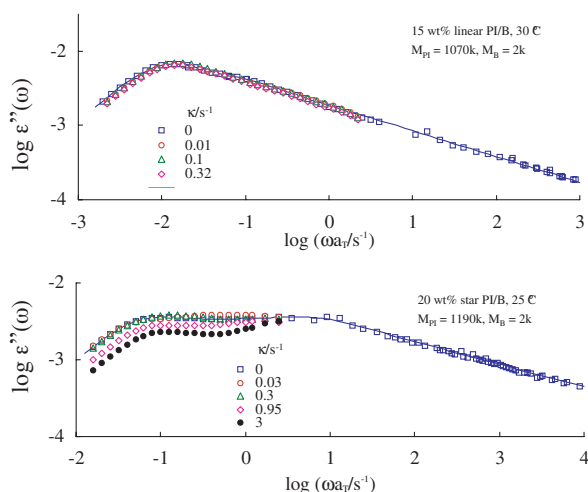
Dielectric Behavior of Entangled cis-Polyisoprene under Fast Shear.

Nonlinear relaxation is the most prominent feature of entangled polymer chains. A convective constraint release (CCR) mechanism, allowing the relaxation through a flow-induced chain motion, plays a central role in a recent molecular model [1]. This model describes the nonlinear viscosity (η) data fairly well, but the CCR picture assumed in the model has not been tested.

For this test, the dielectric loss $\epsilon''(\omega)$ was measured at various angular frequencies ω for linear and six-arm star cis-polyisoprene (PI) chains under fast shear [2]: For these type-A chains, the dielectric relaxation frequency ω_e and relaxation intensity $\Delta\epsilon$ reflect the frequency of global chain motion and the chain size in the shear gradient direction, respectively.

For solutions of the PI chains in an oligomeric butadiene (B), the η data strongly decreased with increasing shear rate κ above the ω_e at equilibrium ($= 0.01 \text{ s}^{-1}$ and 0.08 s^{-1} for the linear and star PI). However, the ϵ'' data demonstrate just weak κ dependencies of ω_e and $\Delta\epsilon$ in particular for the linear PI; see Figure. The weak dependence of the chain size, seen through the $\Delta\epsilon$ data, is attributed to a flow-induced orientational cross-correlation of the chain segments expected from the CCR picture [2]. However, the flow-induced acceleration of the chain motion (proportionality between κ and ω_e) deduced from the simplest CCR picture is not observed experimentally. Thus, the current CCR model needs to be further refined.

1. S.T. Milner, T.C.B. McLeish, and A.E. Likhtman, *J. Rheol.*, **45**, 539 (2001).
2. H. Watanabe, S. Ishida, and Y. Matsumiya, *Macromolecules*, **35**, 8802 (2002).



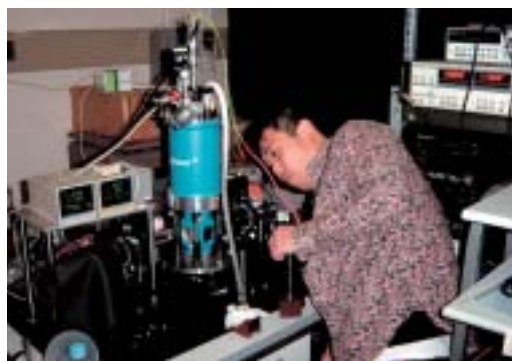
Dielectric loss of entangled cis-polyisoprene under shear flow. Upper panel: linear polyisoprene, lower panel: six-arm star polyisoprene. Dielectric loss of star polyisoprene at low frequencies is significantly suppressed by fast shear flow.

Electric Birefringence of amorphous polymers around the glass transition zone.

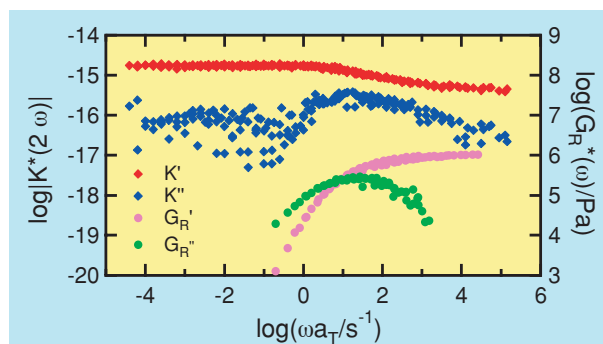
Amorphous polymers become anisotropic and birefringent when they are deformed. Reducing the strain induced birefringence is an important problem in processing of optical devices such as lenses and optical memory discs. We have shown that the strain induced birefringence can be related to the stress by the modified stress-optical rule, MSOR. The essence of the MSOR is the two molecular mechanisms (the chain orientation and twisting of the repeating units) that cause the birefringence.[1]

The MSOR is useful to understand the molecular dynamics of polymers around the glass transition zone.[2] Recently, we have measured electric birefringence of bulk polystyrene under oscillatory field. Comparing the chain orientation component of the shear modulus, we have found that the relaxation of the electric birefringence is mostly originated from chain reorientation. Thus, we have consistently explained all the relaxation processes of the electric birefringence, strain-induced birefringence, and modulus. The present result is easily extended to the reorientation of chain in the magnetic field, which is one of hot topics in the recent polymer science.

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



Measurement of electric birefringence by using a homemade apparatus.



Complex Kerr coefficient, $K^* = K' + iK''$, and chain orientation component of the shear modulus, $G_R^* = G_R' + iG_R''$, for bulk polystyrene ($M = 1050$). G_R^* was determined with the MSOR. Reference temperature is 298.15K.

Fundamental Material Properties

- Polymer Materials Science -

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



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Prof Barbara J Gabrys, The Open University, UK, 7–24 June 2002

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 2002)

Presentations

Hierarchical Structure of Polymer Gels (invited), Kanaya T, Annual Meeting, the Society of Fiber Science and Technology, Japan, Tokyo, 22 May.

Crystallization of Syndiotactic Polypropylene under Shear Flow, Fukushima H, Ogino Y, Kanaya T, Nishida K, Kaji K, Annual Meeting, the Society of Fiber Science and Technology, Japan, Tokyo, 22 May.

Crystallization of Isotactic Polypropylene under Shear Flow, Ogino Y, Fukushima H, Kanaya T, Nishida K, Kaji K, Annual Meeting, the Society of Fiber Science and Technology, Japan, Tokyo, 22 May.

Observation of Speckle during Gelation Process of Poly(vinyl alcohol) Solutions, Takahashi N, Kanaya T, Nishida K, Kaji K, Annual Meeting, the Society of Fiber Science and Technology, Japan, Tokyo, 22 May.

Spinodal Decomposition Type Crystal Nucleation of Polymers, Kaji K, Nishida K, Imai M, Matsuba G, Kanaya T, International Symposium on Polymer Crystallization, Mishima, 9 - 12 June.

Homogeneous Polymer Crystallization with Microphase Separation, Nishida K, Kaji K, Konishi T, Kanaya T, Matsuba G, International Symposium on Polymer Crystallization, Mishima, 9 - 12 June.

Crystallization of Isotactic and Syndiotactic Polypropylenes under Shear Flow, Kanaya T, Fukushima H, Ogino Y, Nishida K, Kaji K, International Symposium on Polymer Crystallization, Mishima, 9 - 12 June.

Similarity between Gels and Glasses in Speckle, Takahashi N, Kanaya T, Nishida K, Kaji K, ISSP Meeting on Properties of Glasses and Glass Transition, Kashiwa, 10 July.

Bamboo Leaf Morphology of Isotactic Polypropylene Crystals, Konishi T, Nishida K, Kanaya T, Kaji K, Polymer Symposium [Kobe], the Society of Polymer Science, Japan, Kobe, 12 July.

Thermal Neutron Spin Echo Measurements on Dynamics of Polybutadiene near Glass Transition, Kanaya T, Watanabe H, Tsukushi I, Kakurai K, 3rd Workshop on Non-equilibrium Phenomena in Supercooled Fluids, Glasses, and Amorphous Materials, Pisa, 22 - 27 September.

Studies on Polymer Crystallization by Synchrotron Radiation, Kanaya T, Fukushima H, Ogino Y, Takahashi N, Nishida K, Kaji K, Autumn Meeting, the Society of Polymer Science, Japan, Fukuoka, 2 - 4 October.

Origin of Viscosity of Polyelectrolyte Solutions & Control of Higher Order Structures of Polymer Materials by a Rapid Temperature Jump Method (invited), Nishida K, 59th Symposium for Young Polymer Scientists, the Society of Polymer Science, Japan, Sakai, 16 November.

Gelation of Poly(vinyl alcohol) under Shear Flow, Takahashi N, Kanaya T, Nishida K, Nagao M, Takahashi Y, Autumn Meeting, Jpn. Soc. Neutron Sci., Kumatori, 9 December.

Grants

Kanaya T, Fukao K, Imai M, Nishida K, Preparatory mechanism of polymer crystallization, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2003.

Crystallization of Polymer Melts under Flow

Real time reo-DPLS and reo-SAXS

Crystallization of polymer melts under flow has been extensively studied because in most polymer processing operations such as extrusion, injection molding and fiber spinning, the molten polymers are exposed to various flows. Polymer chains are oriented under flow and crystallize with morphologies different from those under quiescent condition: the so-called shish-kebab structure. In such structure, extended chains in the direction of the applied flow act as row-nuclei (shish) and chain folded lamellae (kebab) grow on the shish in a direction perpendicular to the extension axis.

In this work we have investigated crystallization process of isotactic polypropylene (iPP), syndiotactic polypropylene (sPP) and polyethylene (PE) under flow using depolarized light scattering (DPLS), small-angle X-ray scattering (SAXS), and small-angle neutron scattering (SANS) techniques to elucidate formation mechanism of shish-kebab structure.



Photo: Ogino, Y.
working on reo-DPLS
instrument.

After keeping a sample at a given temperature above the melting temperature, it was cooled down to a given annealing (or crystallization) temperature, and just after reaching the temperature, a step shear was applied to the sample for a given duration, and then time-resolved DPLS and SAXS measurements were started.

Fig. 1 shows 2D DPLS pattern during crystallization process of iPP at 132 °C after a step shear. After an induction period before nucleation, a weak but sharp streak appears in a direction perpendicular to the shear flow, suggesting that shish structure appears along the flow direction. After the shish formation, kebab structure appears in time resolved SAXS pattern as shown in Fig. 2 where two spots along the flow direction are clearly observed, corresponding to a long period of the kebab structure.



Fig. 1. 2D DPLS pattern of iPP at 1'57'' after shear.

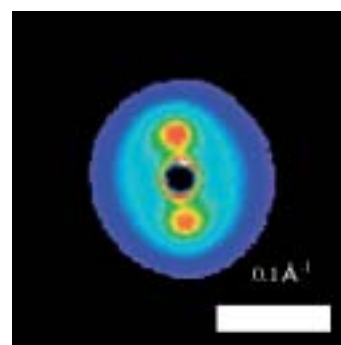


Fig. 2. 2D SAXS pattern of iPP at 4'22'' after shear.

Reo-SANS

SANS measurements were also performed on elongated deuterated PE (Mw = 200,000) including a small amount of protonated PE (Mw = 2,000,000). As seen in Fig. 3, shish-kebab structure was clearly observed in 2D SANS pattern, suggesting that the shish-kebab structure formation is enhanced by the ultra-high molecular weight PE.

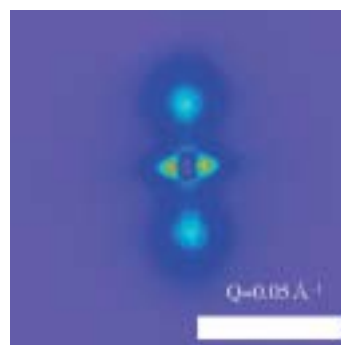


Fig. 3. 2D SANS pattern of elongated PE mixture (see text).

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, Ebisawa T, Tasaki S, Glass transition mechanism of polymers, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

Kanaya T, Nano-assembly of polymers by neutron spin echo, Grant for Researches at Dawn, Japan Atomic Energy

Research Institute, 7 October 2002 - 31 March 2003.

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.

Awards

Kanaya Toshiji, SFSTJ Award, Hierarchic Structure of Polymer Gels, The Society of Fiber Science and Technology, Japan, 22 May 2002.

Fundamental Material Properties - Molecular Dynamic Characteristics -

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Prof HU, Shaohua

Donghua University, China, 15 January–23 March, 2002

Dr AMORNSAKCHAI, Taweechai

Mahidol University, Thailand, 1 April–31 May, 2002

Dr SCHELER, Ulrich

Institut fuer Polymerforschung, Dresden e. V., Germany, 27–28 November, 2002

Scope of Research

The research activities in this subdivision cover structural studies and molecular motion analyses of polymers and related low molecular weight compounds in the crystalline, glassy, liquid crystalline, solution, and frozen solution states by high-resolution solid-state NMR, dynamic light scattering, electron microscopy, X-ray diffractometry, and so on, in order to obtain basic theories for the development of high-performance polymer materials. The processes of biosynthesis, crystallization, and higher-ordered structure formation are also studied for bacterial cellulose.

Research Activities (Year 2002)

Presentations

Structural Study of Microbial Poly(ϵ -lysine) in the Different States, Horii F, Masuda K, Nakamura H et al., 224th ACS Annual Meeting, 20 August.

Critical Fluctuations and Dissipative Structure Formation in Solution of Cellulose Acetates in Couette Flow (Paris, France), International Conference on Theor. Phys., Tsunashima Y, International Union for Pure and Appl. Phys., 24 July.

Chain Dynamics and Structure Transition of Cellulose Acetates in Dilute Solution (Kyoto), IUPAC Polym. Conference, Tsunashima Y, Soc. Polym. Sci., Jpn., 4 December.

Structure of Band-like Cellulose Assemblies Produced by *Acetobacter Xylinum*, Hirai A, Tsuji M, Horii F, 1st International Cellulose Conference, 6 November.

Structure and Dynamics of Disordered Polymers and their Properties, Kaji H, 1st RIKEN Symposium “Structural and Functional Aspects of Polymer Crystals”, 19 July.

Dynamic Assemblies of Cellulose Acetates in Polar Sol-

vents, Tsunashima Y, Kawanishi H, Mizuno M, Onodera G, Horii F; Structure of Band-like Cellulose Assemblies Produced by *Acetobacter Xylinum* as Revealed by TEM and X-Ray Diffraction Analysis, Hirai A, Tsuji M, Horii F; Characterization of Specific Interactions in Polymers by an MAS NMR Method Without Irradiating Passive Spins, Kaji H, Horii F, 6th International Conference of ICRIS'02 (Kyoto), 31 January.

Solid-Phase Reaction and Microfibril Structure of Bacterial Cellulose, Yamamoto H, Horii F, Hirai A, Annual meeting, Cellulose Soc. Jpn, 11 July.

Studies on Unique Thermal Changes in Conformation for Atactic Polypropylenes, Nishimura T, Kuwabara K, Kaji H, and Horii F, Annual Meeting, Soc. Polym. Sci., Jpn., 29 May.

The Analysis of Dynamics in Amorphous Super-Engineering Plastics by Two-Dimensional Solid-State NMR Spectroscopy, Kaji H, Okazaki H, Fuke K, Horii F, Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 4 October.

Selective Observation and Quantification of Amorphous Trans Conformers in PET by Zero-Quantum MAS Solid-State NMR

We present a new NMR method for identifying and quantifying conformations of ^{13}C -labeled polymers under magic-angle spinning (MAS). The experiment is based on zero-quantum (ZQ) dephasing under the recoupled chemical-shift anisotropy (CSA), and the observed magnetization is dephased by the relative orientation of relevant two ^{13}C sites. This method is applied to the $\text{O}-^{13}\text{C}_2-^{13}\text{C}_2-\text{O}$ moieties in amorphous poly(ethylene terephthalate) (PET). Signals of near-trans conformations decay more slowly than those near gauche, which permits the determination of trans : gauche ratio and torsion angles of respective components. This experiment also enables selective observation of amorphous trans component, which cannot be detected by traditional CP/MAS experiments due to complete overlap with dominant gauche signal. The angular resolution is especially high for near-trans conformations. From the decay curves (see Fig. 1), it is determined that the trans fraction is $12 \pm 3\%$ and the torsion angle is distributed with a standard deviation $\sigma_\psi = 16^\circ$ around the ideal trans state $\psi_{\text{ave}} = 180^\circ$ for amorphous PET.

In semicrystalline PET (not shown here), the crystalline

trans : crystalline gauche : amorphous trans : amorphous gauche = 23 : 0 : 20 : 57 (± 5) %. The trans fraction in the amorphous regions of semicrystalline PET, $26 \pm 5\%$, is found to be significantly higher than $12 \pm 3\%$ in amorphous PET.

The technique presented here opens the possibility of characterizing the conformations of various kinds of ordered and disordered materials, including organic, inorganic, and bio-materials.

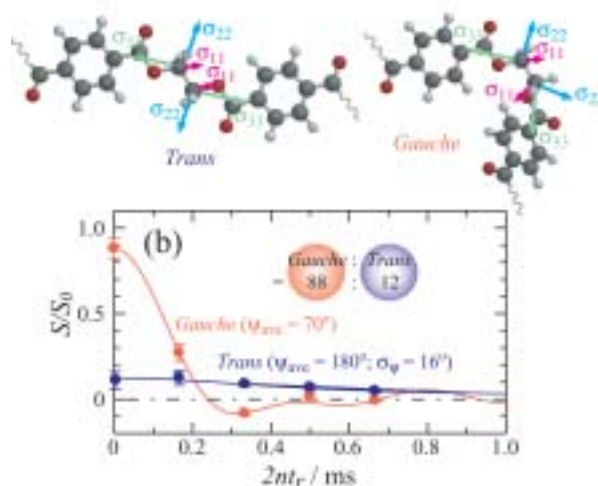


Fig. 1. ZQ-CSA-dephasing curves of amorphous PET. The quantitative torsion angles are determined from the curves.

Hierarchical Structure of Cellulose Produced by *Acetobacter Xylinum*

We have been studying the hierarchical structure formation process of cellulose produced by *Acetobacter xylinum* under various culture conditions. Under standard culture conditions, bacteria produce cellulose gels which are composed of thin ribbon assemblies. A ribbon-like assembly is extruded parallel to the long axis of the cell and twisted in a right-handed manner. In contrast, at 4°C a band-like cellulose assembly, which consists of strand-like cellulose entities, is extruded perpendicularly to the long axis of the bacterial cell. We have been clarifying the role of extensive hydrogen bonding of cellulose and its hydrophobicity on the hierarchical structure formation process of bacterial cellulose. Together with this vital information we are trying to design hybrids based on cellulose at molecular level. This new and revolutionary material, it is hoped, will solve the recent energy and environmental problems facing today's world.

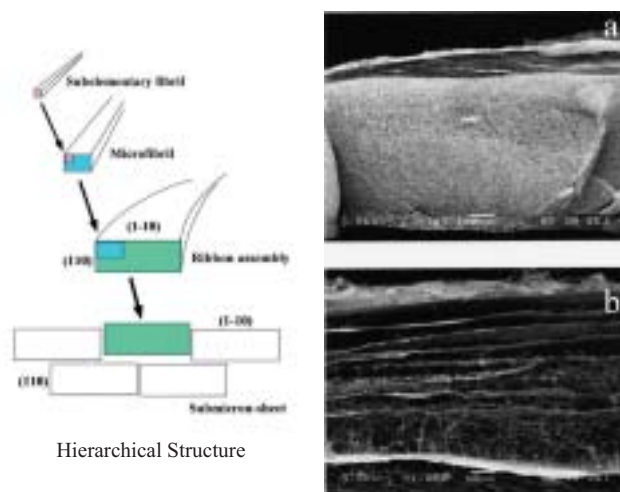


Fig. 2. (a) SEM photo of a freeze-dried cellulose gel sample. (b) Magnified image near the surface of (a). Stacked submicron sheets (see the left model) are observed.

Analyses of Local Structures in Glassy Polymers by Multiple-Quantum NMR Methods, Kaji H, Horii F, Schmidt-Rohr K (Iowa State Univ.), NMR Conf. Jpn., 8 November.

Grants

Horii F, Multi-Dimensional Structure Control of Microbial Polymers in the Biosynthesis Process and Precise Analysis of their Structure and Functionality, Grant-in-Aid for Scientific Research (C)(1), 1 April 2002 - 31 March 2003.

Hirai A, Molecularly Aggregated State of Bacteria-Produced Cellulose Made Through Nano-Spinning, Grant-in Aid for Sci-

entific Research (C)(2), 1 April 2001 - 31 March 2003.

Kaji H, Precise Analyses of Polyamorphous Structure and Dynamics by Advanced Solid-State NMR, Grant-in Aid for Young Scientists (A), 1 April 2001 - 31 March 2003.

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

Award

Masuda K, Award for the Outstanding Paper, The Society of Polymer Science, Japan, 30 May.

Organic Materials Chemistry

- Polymeric Materials -

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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 2002)

Presentations

Designing New Surfaces by LRP, Fukuda T, and 3 other presentations, Macro Group UK, International Conference on Polymer Synthesis, UK, 29 Jul - 1 Aug.

Mechanism and Kinetics of LRP: Absolute Comparison of Theory and Experiment, Fukuda T, and 2 other presentations, 224th ACS National Meeting, USA, 18 - 22 Aug.

Functionalization of Cellulosics by LRP, Tsujii Y, and 1 other presentation, 1st International Cellulose Conference, Kyoto, 6 - 8 Nov.

6 Presentations, Spring Meeting, Soc. Polym. Sci, Jpn., 29 - 31 May. 2 Presentations, Polymer Symposium, Soc. Polym. Sci. Jpn., 12 Jul. 6 Presentations, Autumn Meeting, Soc. Polym. Sci, Jpn., 2 - 4 Oct.

Grants

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

Fukuda T, Development of Living Radical Emulsion Polymerization, Grant-in-Aid for Science Research. (B)(2), 1 Apr 2000 - 31 Mar 2003.

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

Tsujii Y, Development of New Surface-Modifying Technology, Ind. Tech. Research Grant Program from NEDO, 1 Nov 2000 - 31 Mar 2003.

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

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

Absolute Comparison of Kinetic Theory and Experiment on Living Radical Polymerizations

Absolute comparison of the kinetic theory and experiment was made for the two main branches of living radical polymerization, i.e., nitroxide-mediated polymerization (NMP) and atom transfer radical polymerization (ATRP). Figure 1 shows an example, in which the theories (lines) and experiment (circles and squares) on the polymerization rate and polydispersity index for NMP are compared. It is an *absolute* comparison, since the parameters appearing in the theoretical formula have all been determined by independent experiments. Experiment well agrees with theory (Figure 1). This is the first experimental evidence showing that the most fundamental parts of the LRP kinetic theories work on an absolute scale. The result also demonstrates that the addition of conventional initiator such as benzoyl peroxide can not only increase the polymerization rate but also lower the polydispersity, as is predicted by the theory. Similar results were obtained for ATRP, too. The kinetic knowledge obtained in this work is important to design experimental conditions for the highest possible achievement.

Glass Transition Temperatures of High-Density Poly(methyl methacrylate) Brushes

Polymers densely end-grafted on a solid surface will be obliged to stretch away from the surface, forming a so-called “polymer brush”. We were the first to succeed in applying atom transfer radical polymerization (ATRP), a variant of living radical polymerization, to the graft polymerization on a solid surface and yielding a polymer brush composed of low-polydispersity polymer with the highest graft density reported to data (ca. 0.7 chains/nm²). It was previously revealed that in such a graft layer polymer chains were highly extended in a good solvent, nearly to their full length, and the properties of this high-density polymer brush in a good solvent condition are quite different and unpredictable from those of “moderately dense” polymer brushes. However, the properties of this high-density polymer brush in dry state have rarely been characterized. We studied the glass transition temperature (T_g) of the high-density polymer brush for the first time. It was revealed that T_g of the high-density polymer brushes is quite different from that of the cast (ungrafted) films and the difference originates from the characteristic bulk structure/properties of the high-density brushes.

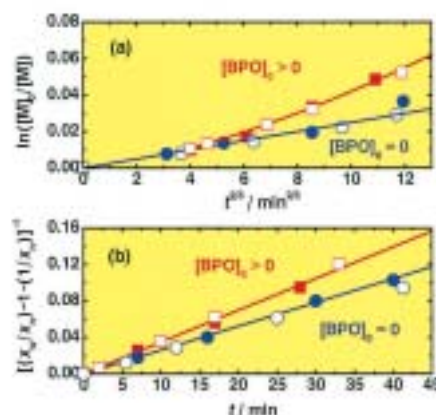


Figure 1. Plot of (a) $\ln([M]_0/[M])$ vs $t^{1/2}$ and (b) $[(x_w/x_n) - 1 - (1/x_n)]^{-1}$ vs t for the styrene/PS-DEPN/(BPO) systems (80 °C): $[PS-DEPN]_0 = 25$ mM; $[BPO]_0 = 0$ (● and ○) and 4.7 mM (■ and □), where M is monomer (styrene), PS is polystyrene, DEPN is *N-tert*-butyl-1-diethylphosphono-2,2-dimethylpropyl nitroxide, BPO is benzoyl peroxide, and x_w and x_n are weight- and number-average degrees of polymerization, respectively. The duplicated experiments (circles and squares) well agree with the theoretical (solid and broken) lines calculated with the independently determined rate constants.

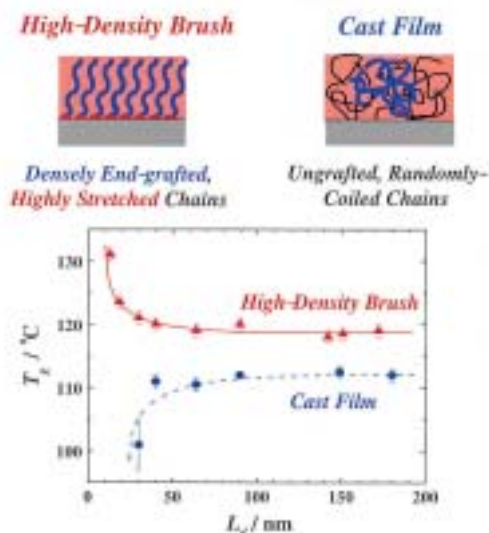


Figure 2. Plots of T_g vs. L_d (film thickness) for the high-density poly(methyl methacrylate)(PMMA) brushes (▲) and the cast (ungrafted) PMMA films (●) measured by temperature-variable spectroscopic ellipsometry. PMMA brushes with a constant graft density (ca. 0.7 chains/nm²) but differing graft chain lengths (the number-average molecular weight, M_n , 15000 < M_n < 182000) were prepared by ATRP on a silicon substrate. The cast PMMA films were also prepared on a silicon substrate. The brush and the cast film with nearly the same film thickness have almost the same molecular characteristics. Therefore, the T_g difference between these two types of films arises only from the difference in their film structure.

Organic Materials Chemistry

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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 π -conjugated systems, particularly the positively charged species stabilized by σ - π interaction; synthesis of new redox-active and supramolecular π -systems; organo-chemical transformation of 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_{60} cation and its application for synthesis of functional materials.

Research Activities (Year 2002)

Presentations

Synthesis of New Fullerene Dimers and Open-Cage Fullerenes by Solid-State and Liquid-Phase Reactions of C_{60} , Komatsu K, Murata Y, et al., The 201st Meeting of the Electrochemical Society, 16 May, Philadelphia, USA.

The Solvent-Free, Solid-State Reaction of Fullerenes to Give Novel Fullerene Dimers, Komatsu K, The 5th International Symposium on Green Chemistry in China, 23 May, Hefei, China.

Radical Cation and Dication of Sulfur-Containing π -Electron Systems Stabilized by Rigid σ -Frameworks, Nishinaga T, Komatsu K, et al., The 5th International Symposium on Functional π -Electron Systems, 1 June, Ulm, Germany.

Fullerene-Based Nanomaterials, Komatsu K, The 12th International Symposium on Supramolecular Chemistry, 7 October, Eilat, Israel.

Structure and Properties of a Novel Fullerene Dimer $RC_{60}-C_{60}R$ and Facile Generation of Fullerenyl Cation RC_{60}^+ , Cheng F, Murata Y, Kitagawa T, Komatsu K, Gordon Research Conference, 29 July, Aioi, Japan.

Grants

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

Kitagawa T, Construction of fullerene-coated nanostructures using alkylfullerenyl cations, Grant-in-Aid for Scientific Research (C) (2), Apr. 2002 - Mar. 2004.

Nishinaga T, Design and synthesis of π -conjugated oligomers folded in helical structure by electron transfer, Grant-in-Aid for Encouragement of Young Scientists (A), Apr. 2002 - Mar. 2004.

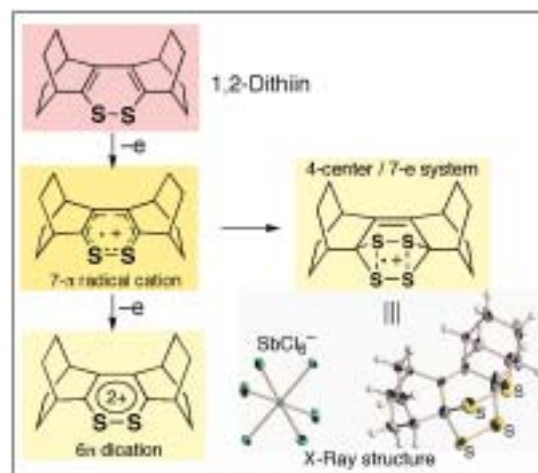
Murata Y, Synthesis of endohedral fullerenes by the use of organic chemistry, Grant-in-Aid for Encouragement of Young Scientists (A), Apr. 2002 - Mar. 2004.

Kitagawa T, Construction of nano-electronic devices based on precise molecular design, CREST, Japan Science and Technology Corporation, Nov. 2002 - Oct. 2007.

Murata Y, Komatsu K, Application of functionalized fullerenes for fabrication of solar cells, Academic-Industrial Cooperative Research Fund, Aug. 2002 - Jul. 2003.

Formation of the First Stable Radical Cation Having a Tetrathia 4-Center/7-Electron Bond

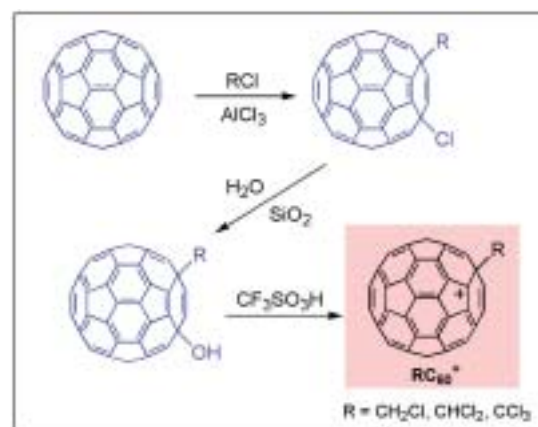
Annulation of cyclic π -conjugated systems with rigid bicycloalkene frameworks has been shown to stabilize the π -system when it is positively charged, both by the σ - π conjugation and steric protection effects. Thus, the radical cation and dication of 1,2-dithiin (1,2-dithia-3,5-cyclohexadiene) were generated as stable species by this structure modification for the first time. Furthermore, the radical cation was found to disproportionate to give a totally new radical cation having the tetrathiabicyclic structure, which is remarkably stabilized by a strong transannular interaction among four sulfur atoms forming a novel 4-center/7-electron system, together with a thiophene derivative.[1]



1. Wakamiya A, Nishinaga T, Komatsu K, *J. Am. Chem. Soc.*, **2002**, 124, 15038.

Generation and Thermodynamic Stabilities of Alkylfullerenyl Cations

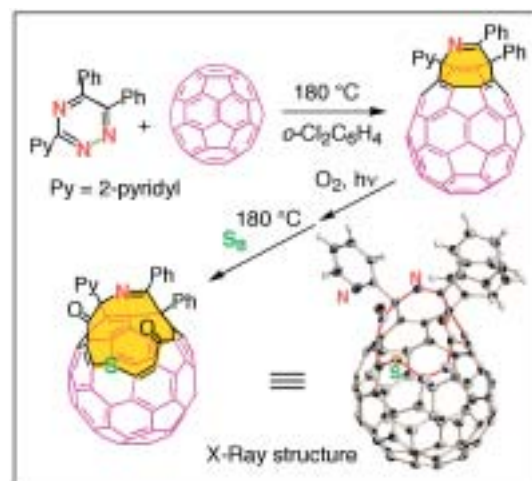
The generation and the direct observation of functionalized fullerenyl cations have been considered a challenging task, owing to the electronegative nature of the C_{60} cage. We could generate monoalkylated fullerenyl cations (RC_{60}^+ , R = chloroalkyl group) as long-lived ions by treating the corresponding fullerene precursors with a strong acid. Spectral analysis showed that these cations have structures with C_s symmetry and their positive charge is mainly located on C-2. Kinetic studies of the S_N1 solvolysis of the corresponding chlorides and the equilibrium constants of the hydrolysis to form fullereneols indicated that the cations RC_{60}^+ have stabilities comparable to that of the *tert*-butyl cation.[2]



2. Kitagawa T, Lee Y, Komatsu K, et al., *Chem. Commun.*, **2002**, 3062.

Synthesis of a Novel Open-Cage Fullerene Derivative with a 13-Membered-Ring Orifice

As the first step in a novel approach to endohedral fullerene complexes, which are expected as nano-scale materials with unique properties, organic synthesis of open-cage fullerenes is quite important. When a thermal reaction of C_{60} with a 1,2,4-triazine derivative was conducted, a [4+2] cycloaddition followed by nitrogen extrusion took place to give a derivative with an 8-membered-ring orifice. This orifice was further enlarged by photochemical oxidation followed by sulfur insertion to the rim of the orifice to give a totally new open-cage fullerene derivative with a 13-membered-ring opening, which is the largest orifice reported so far. A preliminary experiment indicated that it is quite promising to incorporate small molecules into the inside of this fullerene cage.[3]



3. Murata Y, Murata M, Komatsu K, *Chem. Eur. J.*, **2003**, 9, in press.

Synthetic Organic Chemistry

- Synthetic Design -

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Univeriste de Montpellier, 2 July 2002–23 August 2002

Scope of Research

Our research is concerned with some new aspects in the elemento-organic chemistry, including (1) the design and synthesis of novel π -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 σ -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 2002)

Presentations

Boron-Containing π -Electron Systems: Photophysical Properties Control Based on the p_{π} - π^* Conjugation, Yamaguchi S, Shirasaka T, Akiyama S, Tamao K, 5th International Symposium on Functional π -Electron Systems, 30 May - 4 June, 2002, Ulm, Germany.

My 35 Years in Organosilicon Chemistry (F. S. Kipping Award Lecture), Tamao K, The 13th International Symposium on Organosilicon Chemistry, 28 August, Guanajuato, Mexico.

Relationship between Photophysical Properties and Conformation of Oligosilanes, Tsuji H, Terada M, Toshimitsu A, Tamao K, 16th Symposium on Fundamental Organic Chemistry, 4 October, Tokyo, Japan.

Grants

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

Yamaguchi S, Elemento-Organic π -Electron Systems for the Materials Science, PRESTO, Japan Science and Technology Corporation, December 2001 - November 2004.

Awards

Tamao K, Toray Science and Technology Prize, 14 March.

Yamaguchi S, The Chemical Society of Japan Award for Distinguished Young Chemists, Creation of Functional π -Electron Systems Containing Group 13, 14, and 15 Elements, The Chemical Society of Japan, 29 March.

The Disilane Chromophore: Photoelectron and Electronic Spectra of Hexaalkyldisilanes and 1,(n+2)-Disila[n.n.n]propellanes

Photoelectron spectra, solution UV absorption, and magnetic circular dichroism (MCD) of hexamethyldisilane (**1**), hexaethyldisilane (**2**), hexa-tert-butylidisilane (**3**) and the 1,(n+2)-disila[n.n.n]propellanes [**n** = 4 (**4**) and 5 (**5**)] were measured, as was the linear dichroism (LD) of **3** and **4** partially aligned in stretched polyethylene. The results support the assignment of the lowest energy electronic absorption band of the disilanes **1** - **5** to a doubly degenerate σ_{SiSi}^* (HOMO) - π_{SiC}^* (LUMO) transition, and of the next band, observed in the solution spectra of **2** - **4**, and in the gas-phase spectrum of **1**, to a $\sigma_{\text{SiSi}} - \pi_{\text{SiSi}}^*$ transition [1]. MP2/VTZ optimized geometries of **1** - **5** and ab initio calculations of the molecular orbital energies (HF/VTZ//MP2/VTZ) and

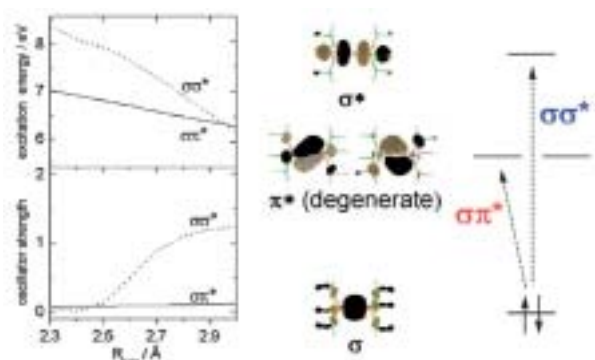


Figure 1. Excitation energy and oscillator strengths of disilane together with their molecular orbitals.

ionization potentials (ROVGF/VTZ//MP2/VTZ) of these disilanes reproduce the reported geometries and the trends observed in the photoelectron spectra, respectively. Calculations of the Kohn-Sham orbital energies (B3LYP/6-31G(d)) and transition energies (TD DFT B3LYP/6-31G(d)) of **1** as a function of Si-Si bond length suggest that many of the trends observed in the UV absorption spectrum of **3**, including the small energy difference between the two transitions observed and the large extinction coefficient of the higher energy ($\sigma_{\text{SiSi}} - \sigma_{\text{SiSi}}^*$) band are due to its very long Si-Si bond.

1. Casher DL, Tsuji H, Sano A, Katkevics M, Toshimitsu A, Tamao K, Kubota M, Kobayashi T, Ottosson H, Michl J, *J. Phys. Chem. A*, in press.

Tamao K, F. S. Kipping Award, The American Chemical Society, 9 April.

Shirasaka T, Symposium Poster Award, 49th Symposium on Organometallic Chemistry, Japan,

Dibenzoboroles as a New Boron-Containing π -Electron Systems

Boron-containing π -electron systems represents a new class of organic materials with intriguing electronic and photophysical properties due to the $p_{\pi} - \pi^*$ conjugation through vacant p-orbital of the boron atom. One notable aspect may be the control of this conjugation which provides an opportunity to modify their properties. In this report, we have succeeded in the synthesis of a series of dibenzoborole derivatives with various groups such as (*N,N*-diphenylamino)phenyl, thienyl, and bithienyl groups at the 3,7-positions and have studied their photophysical properties. These new π -electron systems show significant solvatochromism in the fluorescence spectra (Figure 2a) [2]. Thus, about 100-140 nm blue shifts in the emission maxima and 20-30 fold increments in the quantum yields are observed by changing the solvent from THF to DMF. Similar fluorescent changes are observed upon the addition of *n*-Bu₄NF to their THF solutions, demonstrating their sensing abilities toward a fluoride ion. These fluorescence changes result from the "on/off"-control of the $p_{\pi} - \pi^*$ conjugation in their LUMO by the coordination of donor solvents or fluoride ion to the boron atom in the dibenzoborole skeleton (Figure 2b).

2. Yamaguchi S, Shirasaka T, Akiyama S, Tamao K, *J. Am. Chem. Soc.*, **124**, 8816-8817 (2002).

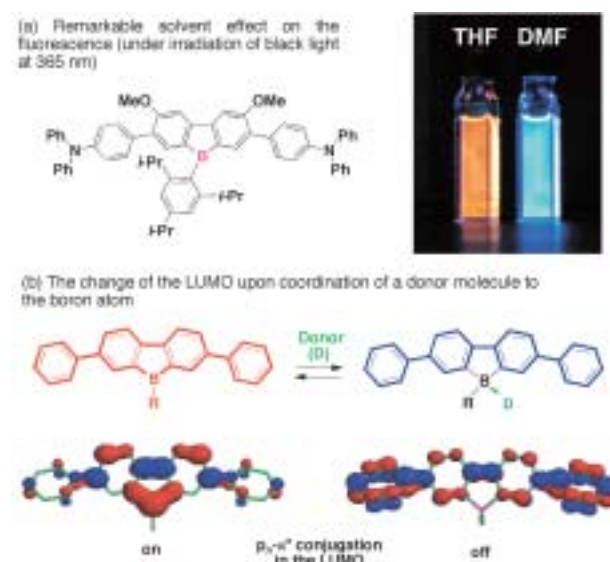


Figure 2. The ON/OFF control of the $p_{\pi} - \pi^*$ conjugation in the dibenzoborole-containing π -electron systems.

Dibenzoborole-Based π -Electron Systems: Synthesis, Photophysics, and Sensing Ability for Fluoride Ion, Kinki Chemical Society, 13 September 2002.

Synthetic Organic Chemistry

- Fine Organic Synthesis -

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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 homo- and heterochiral oligomers.

Research Activities (Year 2002)

Presentations

Asymmetric Synthesis based on Dynamic Chirality of Enolates, Kawabata T, Annual Meeting, Chem. Soc. Jpn., 26 March.

Asymmetric Alkylation of Amino Acid Derivatives under the Control of Aggregation of Enolates, Kawabata T, Kawakami S, *et al.*, Annual Meeting of the Pharmaceutical Society of Japan, 27 March.

Visual Enantiomeric Recognition of Alanine Derivatives, Tsubaki K, Nuruzzaman M, *et al.*, Symposium on Molecular Chirality, 6 June.

Synthesis and Functions of New Homooxa-calix[3]arene Derivatives, Tsubaki K, Maruoka H, Otsubo T, *et al.*, 52th Meeting of the Pharmaceutical Society of Japan (Kinki). 19 October.

Achiral Auxiliaries for Asymmetric Induction, Kawabata T, Öztürk O, *et al.*, 28th Symposium on Progress in Organic Reactions and Syntheses, 5 November.

Synthesis and Functions of Chiral Origo Naphthalene Deriva-

tives, Tsubaki K, Morikawa H, *et al.*, 17th Meeting of Cyclophane Chemistry. 8 November.

Nucleophilic Catalysis in Kinetic Resolution of Racemic Alcohols, Kawabata T, International Symposium on Biotechnology, Metal Complexes and Catalysis, 26 November.

Grants

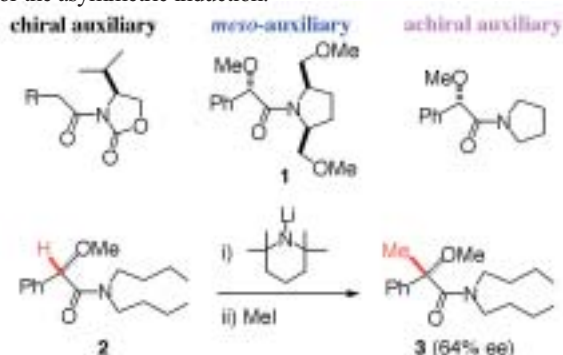
Kawabata T, Asymmetric Synthesis through Nucleophilic Catalysis, Grant-in-Aid for Scientific Research (B) (2), 1 April 1999 - 31 March 2002.

Kawabata T, Development 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.

Achiral Auxiliaries for Asymmetric Induction

Chiral auxiliary is frequently used in asymmetric synthesis. It is still the most reliable and predictable method for the preparation of optically active natural products. It was long believed that auxiliaries have to be chiral to cause any asymmetric induction. However, we found that *meso*-2,5-disubstituted pyrrolidine can be used as an auxiliary for asymmetric induction. For example, methylation of **1** proceeded in 73% ee by treatment with *n*-BuLi/TMEDA in cyclopentyl methyl ether (CPME) followed by addition of methyl iodide. We further found that even achiral amines such as pyrrolidine and dibutyl amine can be used as auxiliaries for asymmetric induction. Treatment of **2** with lithium 2,2,6,6-tetramethylpiperidide in CPME followed by addition of methyl iodide gave **3** in 64% ee in retention of configuration. A mixed aggregate consisting of an achiral enolate and an undeprotonated chiral amide is proposed as a crucial intermediate for the asymmetric induction.

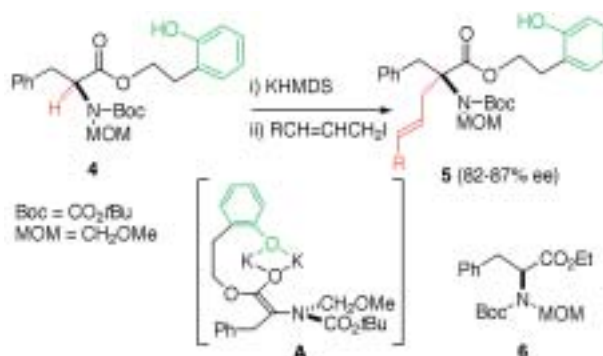


Enantioselective allylation of amino acid derivatives under the control of aggregate structure of chiral nonracemic enolates

Control of aggregation of enolates is one of the long-standing problems in enolate chemistry. Addition of strongly coordinating ligands such as HMPA or TMEDA is a typical approach to this issue. A new approach by formation of intramolecular mixed aggregate with pseudo-enolate subunit is shown here. Enolates usually exist as a mixture of different aggregates in solution, such as the case of an enolate generated from ethyl ester **6**. The complexity of the aggregates often causes difficulties in controlling selectivity of the reactions. Phenylalanine derivative **4** with a phenol group (pseudo-enolate subunit) was designed to form stable intramolecular aggregate **A** as a single aggregate species on treatment with a base.

α -Allylation of **4** proceeded in 82~87% ee, which is greatly improved than that of **6** (23~69% ee). It was also found that

formation of an intramolecular aggregate enhances kinetic stability of a chiral nonracemic enolate against racemization; a half-life to racemization of a potassium enolate generated from **4** is *ca.* ten times as long as that generated from **6**. In both cases, chirality of the starting materials is preserved in the enolate intermediates as C-N axial chirality of a dynamic nature. Optically active α -allylated amino acids are versatile intermediates for functional peptides.



Chromogenic Homooxalix[3]arene Receptor

Homooxalix[3]arene is related to calix[4]arene and 18-crown-6 ether with unique structural features. It has been known, however, that difficulties arose in the transformation of functional groups on the upper rim due to the presence of three fragile dibenzylether linkages. We describe here, for the first time, the introduction of functional groups on the upper rim through successive reactions of **7** (i.e. the Mannich reaction, exhaustive methylation, *p*-quinone methide formation, and nucleophilic substitution) in 45-59% overall yields. The artificial host molecule **9**, consisting of homooxalix[3]arene and pyridinium *N*-phenolate dye (Reichardt dye E_T1) has been prepared. Host **9**, with a proton-ionizable phenol group that acts as chemical switch, causes color change against alkaline metals and various kind of amines.



Award

Tsubaki K, The ICR Award for Young Scientists, Molecular Recognition using Phenolphthalein Derivatives, ICR, 6 Decmber.
Morikawa H, Best Poster Award, Effective Synthesis of Chiral

Origo-Naphthalene Derivative, The Pharmaceutical Society of Japan (Kinki) and the Society of Synthetic Organic Chemistry, Japan (Kansai), 10 December.

Bioorganic Chemistry - Organoelement Chemistry -

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



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Prof Steudel, Ralf

Technical University of Berlin, Germany, 5 April 2002–1 May 2002

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 2002)

Presentations

Chalcogenation reaction of kinetically stabilized doubly bonded systems between heavier group 15 elements, Sasamori T, Takeda N, Tokitoh N, 20th International Symposium on the Organic Chemistry of Sulfur, 14 - 19 July, Flagstaff, USA.

New aspects in the chemistry of silaarenes, Tokitoh N, The 13th International Symposium on Organosilicon Chemistry, 25 - 30 August, Guanajuato, Mexico.

Synthesis, structure, and reactions of the first platinum complexes bearing a disulfur and diselenium ligand, Nagata K, Takeda N, Tokitoh N, 49th Symposium on Organometallic Chemistry, Japan, 12 - 13 September, Kobe.

Synthesis, structure, and reactivities of the first stable

germabenzene, Nakata N, Takeda N, Tokitoh N, 16th Symposium on Fundamental Organic Chemistry, 3 - 5 October, Tokyo.

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), 1 April 2002 - 31 March 2005.

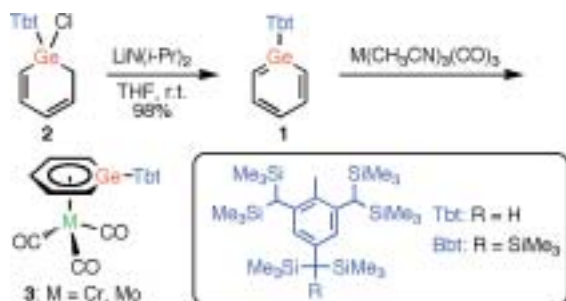
Tokitoh N, Synthesis of dynamic complexes containing heteroatoms by taking advantage of kinetic stabilization, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2002 - 31 March 2006.

Takeda N, Synthesis of novel multiple-bond species of silicon by taking advantage of silylene-isocyanide complexes and

Synthesis and properties of the first stable germabenzene

In recent decades, much attention has been focused on the chemistry of $[4n+2]\pi$ -electron ring systems containing heavier group 14 elements. However, no synthesis and isolation of these compounds as stable molecules had been reported until quite recently due to their extremely high reactivity. We have recently succeeded in the synthesis and characterization of the first stable silabenzene, 2-silanaphthalene, 9-silaanthracene, and 2-germanaphthalene by taking advantage of an efficient steric protection group, Tbt group (*vide infra*). These successful results naturally prompted us to extend this method to the synthesis of a germabenzene, the most fundamental germaaromatic compound having a simple 6 π -electron ring system.

The first stable germabenzene **1** was successfully synthesized by the reaction of the corresponding chlorogermane **2** with $\text{LiN}(i\text{-Pr})_2$ in THF. Although the structural and spectroscopic data and theoretical calculations showed that **1** had aromaticity, in the reactions with MeOH, MesCNO, styrene, phenylacetylene, and 2,3-dimethyl-1,3-butadiene, **1** underwent 1,2- and/or 1,4- addition to the 1-germabuta-1,3-diene moiety reflecting the extremely high reactivity of the Ge–C double bond.



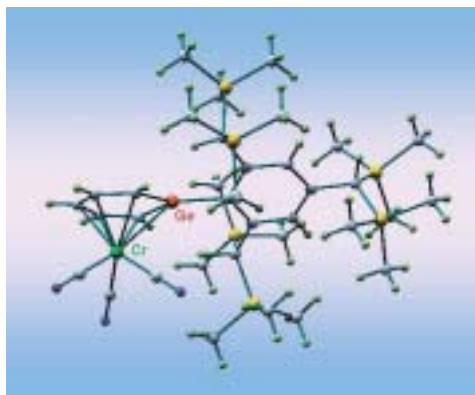
The reactions of **1** with $\text{M}(\text{CH}_3\text{CN})_3(\text{CO})_3$ [M = Cr, Mo] gave the corresponding η^6 -germabenzene complexes of group 6 metals **3**. These results are very interesting because **3** is the first η^6 -germabenzene complexes and these reactions are the first examples showing the aromatic character of germabenzene from the viewpoint of reactivity.

their properties, Grant-in-Aid for Young Scientists (B), 1 Apr 2001 - 31 March 2003.

Awards

Hirano T, Best Poster Presentation Award, Analysis of carbon, hydrogen, and nitrogen contents in silicon-containing compounds using YANACO CHN-CORDER MT-5, The Association of Organic Micro-analysis, 10 May 2002.

Sasamori T, Takeda N, Tokitoh N, The Best Article of the Month, Syntheses, structures and properties of kinetically stabilized distibenes and dibismuthenes, novel doubly bonded sys-



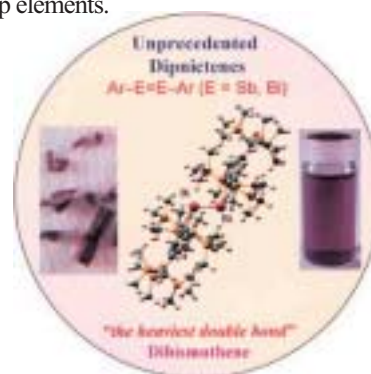
X-ray Structural Analysis of **3**

Synthesis, structures, and properties of novel doubly bonded systems between heavier group 15 elements

Recently, there has been much interest in compounds with a double bond between heavier group 15 elements.

The first stable distibenes and dibismuthenes were successfully synthesized by taking advantage of efficient steric protection groups, Tbt and Bbt groups. The crystallographic analysis, and spectroscopic studies of these stable dipnictenes and theoretical calculations of model compounds led to the systematic comparison of structural parameters and physical properties for all homonuclear doubly bonded systems between heavier group 15 elements.

In addition, condensation of Mes^*PH_2 (Mes = 2,4,6-*tert*-butylphenyl) with BbtBiBr_2 using 1,8-diazabicyclo[5.4.0]undec-7-ene as a base afforded the first stable phosphabismuthene $\text{Mes}^*\text{P}=\text{BiBbt}$, which is also the first stable double-bond compound between the third and sixth row main group elements.



tems between heavier group 15 elements, The Chemical Society of Japan, 25 September 2002.

Shinohara A, Symposium Poster Award, 7th Symposium of the Society of Silicon Chemistry, Japan, Synthesis and properties of kinetically stabilized 1-silanaphthalene, the Society of Silicon Chemistry, Japan, 16 November 2002.

Yamanaka R, Best Presentation Award, The 6th Japanese Symposium on the Chemistry of Biocatalysis, Light-mediated regulation of asymmetric reduction of ketones, Group Biocatalyst Chemistry Japan, 12 December 2002.

Bioorganic Chemistry

- Bioactive Chemistry -

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



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TAKEUCHI, Toshihide (UG)

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 2002)

Presentations

Influence of amino acid numbers between two ligand cysteines of zinc finger proteins on affinity and specificity of DNA binding, Nagaoka M, Kondo Y, Sugiura Y, Annual meeting, Pharm. Soc. Jpn., 27 March.

Design and function of Cys₂His₂-type zinc finger proteins, Sugiura Y, 29th symposium on biological molecular sciences, 12 July.

Design of novel zinc finger peptide recognizing complementary strand, Shiraishi Y, Nagaoka M, Sugiura Y, 6th European conference on bioinorganic chemistry, 1 August.

Engineering of a novel metalloprotein with the conserved residues of Cys₂His₂-type zinc finger, Hori Y, Sugiura Y, 6th European conference on bioinorganic chemistry, 1 August.

Oligoarginine-mediated delivery of bioactive peptides into cells, Futaki S, Nakase I, Niwa M, Suzuki T, Nameki D, Kodama E, Matsuoka M, Sugiura Y, 39th Japanese peptide symposium, 17 October.

Grants

Sugiura Y, Development of order-made type artificial restriction enzymes and repressors, Grant-in-Aid for University and Society Collaboration, 1 April 2000 - 31 March 2003.

Sugiura Y, Regulation of cellular gene function by novel DNA bending finger, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 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, Design of membrane-current regulatory systems using assembly modulation of transmembrane peptides by extramembrane signals, Grant-in-Aid for Scientific Research on the Priority Area of Molecular Synchronization for the Design of New Materials, 1 April 2001 - 31 March 2003.

Futaki S, Creation and intracellular delivery of novel peptides for the regulation of transcription, Grant-in-Aid for Scientific Research (B) (2), 1 April 2000 - 31 March 2003.

Novel Strategy for the Design of New Zinc Finger: Creation of Zinc Finger for AT-Rich Sequence by α -helix Substitution

A novel strategy for the design of a zinc finger peptide on the basis of α -helix substitution has been demonstrated (Figure 1). Sp1HM is a helix-substituted mutant for the wild-type Sp1(zf123) and its α -helix of each finger is replaced by that of fingers 4-6 of CF2-II. The circular dichroism spectrum of Sp1HM suggests that Sp1HM has an ordered secondary structure similar to Sp1(zf123). From the analyses of the DNA binding affinity and specificity by gel mobility shift assay, it is clearly indicated that Sp1HM specifically binds to the AT-rich sequence (5'-GTA TAT ATA-3') with 3 nM dissociation constant (Figure 2). Moreover, the zinc finger peptides for the sequence alternating between the AT- and GC-rich subsites can also be created by the α -helix substitution. This strategy is evidently effective and is also more convenient than the phage display method. Consequently, our design method is widely applicable to creating zinc finger peptides with novel binding specificities.

M. Nagaoka, Y. Doi, J. Kuwahara, Y. Sugiura, *J. Am. Chem. Soc.*, **124**, 6526-6527 (2002).

Basic-Peptide Mediated Protein Delivery into Living Cells

A basic peptide derived from HIV-1 Tat has been reported to have the ability to translocate through the cell membranes and to bring exogenous proteins into the cells. We have demonstrated that these features were observable among many arginine-rich peptides including octaarginine (Arg)₈, and the presence of a ubiquitous internalization mechanism for arginine-rich oligopeptides has been suggested [1]. Branched-chain arginine peptides were also found to translocate through the cell membranes, which suggested the importance of arginine cluster for the internalization [2]. Among the branched-chain peptides examined, the peptide having eight arginine residues showed the most efficient translocation. The charge-dependent way of internalization was basically similar to that observed for the linear oligoarginine peptides. The above findings would provide new insights on the translocation of arginine-rich peptides and on the design of carrier peptides for intracellular protein delivery.

1. T. Suzuki, S. Futaki, M. Niwa, S. Tanaka, K. Ueda, Y. Sugiura, *J. Biol. Chem.*, **277**, 2437-2443 (2002).
2. S. Futaki, I. Nakase, T. Suzuki, Y. Zhang, Y. Sugiura, *Biochemistry*, **41**, 7925-7930 (2002).

Figure 1

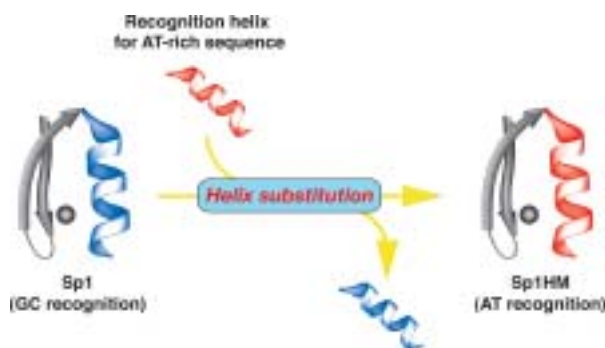
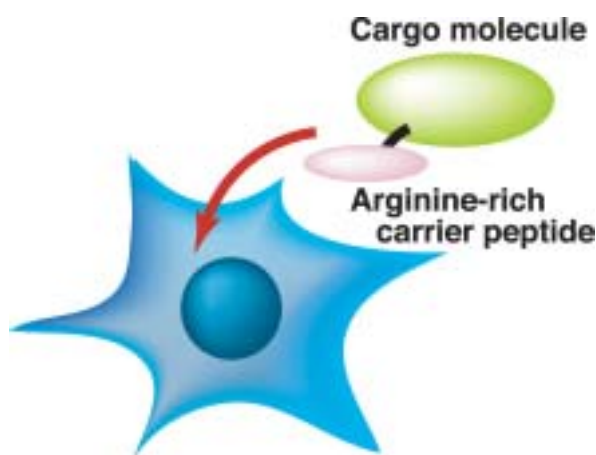
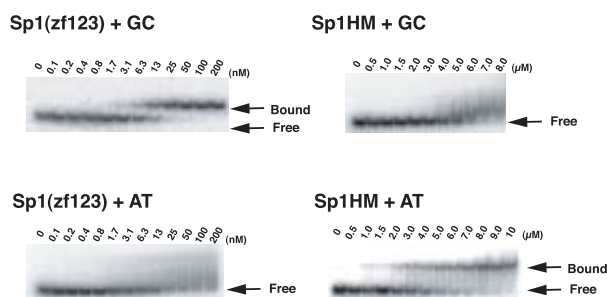


Figure 2



Bioorganic Chemistry

- Molecular Clinical Chemistry -

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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 cancer and neurodegenerative disorders including Alzheimer's disease.

Research Activities (Year 2002)

Presentations

Trp-P-1 and Trp-P-2 modulate the activity of poly(ADP-ribose) synthetase in vitro., Ueda, K., Banasik, M., Stedeford, T., and Price, D. J., 41st Annual Meeting of the Society of Toxicology, Nashville, 18 - 21 March.

Allowable chemical emissions derived from dose-response curves: Solvents as a source of confounding., Banasik, M., Ueda, K., and Stedeford, T., 12th Annual Meeting of the Society of Environmental Toxicology and Chemistry, Vienna, 12 - 16 May.

Trans-activation of E-cadherin gene by a RING-finger protein, LUN., Oyanagi, H., Gorin-Rivas, M. J., Chu, D., Miyahara, R., Yanagihara, K., Tanaka, H., Adachi, Y., Ueda, K., and Wada, H., 8th Central European Lung Cancer Conference, Vienna, 1 - 4 September.

A role of poly(ADP-ribosyl)ation in cell death and its regulation., Tanaka, S., Takehashi, M., Iida, S., Miwa, S., Yamasaki, K., Komeda, M., Ueda, K., 75th Annual Meeting, Jpn. Biochem. Soc., Kyoto, 14 - 17 October.

Dinucleotide repeats in monoamine oxidase A gene associated with Alzheimer's disease and Lewy body variant., Takehashi, M., Tanaka, S., Masliah, E., and Ueda, K., 18th International Congress of Clinical Chemistry and

Laboratory Medicine, Kyoto, 20 - 25 October.

Advanced techniques of gene diagnosis: Non-PCR amplification., Ueda, K., 7th Asian Congress of Clinical Pathology, Kaohsiung, 6 - 9 December.

Grants

Ueda K, Special Coordination Funds for Promoting Science and Technology from the Ministry of Education, Culture, Sports, Science and Technology, 1 April 1998 - 31 March 2003.

Ueda K, Studies on diagnostic characteristics of gene testing and on the systematic reviewing of data with criteria for utility evaluation, Grant-in-Aid for Scientific Research (C), 1 April 2002 - 31 March 2003.

Tanaka S, Suppression of neuronal cell death by poly(ADP-ribose) synthetase inhibitors, Japan Foundation for Applied Enzymology, 1 April 2002 - 31 March 2003.

Intercalation activating fluorescence DNA probe and its application to homogeneous quantification of a target sequence by isothermal sequence amplification in a closed vessel

We developed a completely homogeneous and isothermal method of detecting RNA sequences and demonstrated ultra-rapid and direct quantification of pathogenic gene expression with high sensitivity. The assay is based on isothermal amplification of RNA sequence in the presence of our novel DNA probe, an INAF probe, and measurement of the fluorescence intensity of the reaction mixture. Upon detection of *mecA* gene expression in methicillin-resistant *Staphylococcus aureus* (MRSA), we could quantify initial copies ranging from 10 to 10⁷ copies within 10 minutes. The primer sequences were designed to bind to secondary-structure-free sites of the target RNA, which enabled a totally isothermal protocol to quantify mRNA specifically in a sample of existing genomic DNA. When we applied this method to quantifying the expression of marker genes of *Vibrio parahaemolyticus* and *Mycobacterium bovis*, BCG strain, the results correlated well with the viability of each bacterium. We also demonstrated monitoring *Pab* gene expression of *M. bovis* BCG during cultivation with antibiotics. The present method can potentially realize rapid antimicrobial susceptibility testing of slowly growing organisms, such as tuberculosis.

Ref. Ishiguro, T., *et al.* Anal. Biochem., in press.

A possible role of poly(ADP-ribose) synthetase in neuronal degeneration

Alzheimer's disease (AD) is the most popular neurodegenerative disorder among aged people. A β amyloid deposition is characteristic of AD brain, but its etiological role remains to be clarified. Poly(ADP-ribose) is a polymer synthesized from NAD on proteins in the nucleus of eucaryotic cells. The synthetase (PARS) requires DNA strand termini for its activity, undergoes extensive automodification, and serves as a final target of the caspase cascade in apoptosis.

In view of a concept that neuronal degeneration is a form of apoptosis, we investigated a possible role of PARS in AD pathogenesis. We observed abundant apoptosis of neuronal cells, but rarely glial cells, after treatment with A β peptide or NAC (non-A β component of AD amyloid; a fragment of α -synuclein) (Fig.1). Immunostainings with anti-PARS and anti-poly(ADP-ribose) antibodies revealed that both the enzyme and its product were distributed in the cytoplasm rather than in the nucleus of apoptotic cells.

These results, together with a finding of ROS (reactive oxygen species) production by amyloids, suggest that PARS is automodified upon ROS-induced DNA damage and cleaved by caspase, whereby losing nuclear localization and function, which eventually leads to the cell death.

Ref. Tanaka, S., *et al.* J. Neurochem. 82(2), 305-315 (2002).

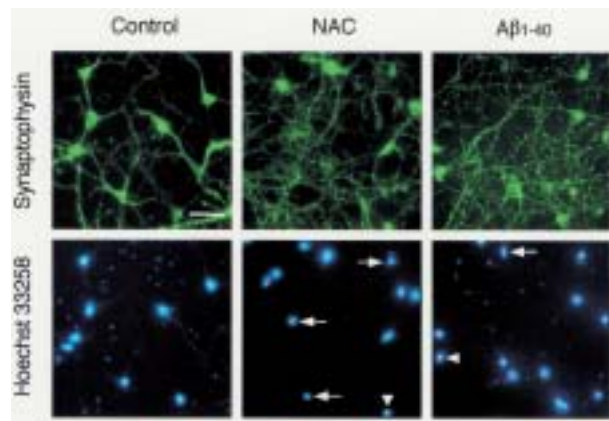


Figure 1. Induction of neuronal apoptosis by amyloid fibrils.

Cortical neurons were double-stained with anti-synaptophysin antibody and Hoechst 33258 after a 24-h incubation with 10 μ M NAC or A β 1-40 fibrils. Representative cells with condensed chromatin (arrow-head) or fragmented nucleus (arrow) are indicated. (Scale bar = 10 μ m)

Dinucleotide repeats in monoamine oxidase A gene associated with Alzheimer's disease and Lewy body variant

Monoamine oxidase (MAO) is one of the primary enzymes regulating metabolism of biogenic amines. Two distinct isoforms of the enzyme, MAOA and MAOB, have different substrate and inhibitor specificities. These enzymes are reportedly involved in the pathogenesis of Parkinson's disease (PD) through the production of oxygen radicals from catabolism of dopamine and activation of exogenous neurotoxins, such as MPTP and its analogues. The association of MAOA and MAOB gene polymorphisms with PD remains to be elucidated. Involvement of MAO in the pathogenesis of Alzheimer's disease (AD) has also been reported. However, allelic association of MAOA and MAOB genes with AD has not been rigorously analyzed.

In this study, we determined the association between (GT)_n dinucleotide repeats in MAOA and MAOB gene loci and PD, pure AD, and Lewy body variant (LBV) of AD. MAOA-GT polymorphisms were significantly associated with pure AD and LBV. MAOA-GT allele 113 was excessively represented in pure AD and LBV compared with controls. Furthermore, the frequency of females homozygous for MAOA-GT allele 113 was higher in pure AD or LBV than controls by 2.8-fold. In contrast, there was no association between MAOA-GT or MAOB-GT polymorphisms and PD. These results suggest that polymorphisms within the MAOA gene may have implication in AD pathology shared by pure AD and LBV.

Ref. Takehashi, M., *et al.* Neurosci.Lett. 327(2), 79-82 (2002).

Molecular Biofunction

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Visitor

Dr ZHAN, Zhengzhu

Anhui Agricultural University, China, 1 October 2001–30 September 2002

Scope of Research

Using various techniques of Natural Product Chemistry, Organic Synthetic Chemistry, Biochemistry as well as Molecular Biology, we are trying to clarify, on molecular basis, various biological events during life cycles where many kinds of biocatalysts (enzymes) are concerned. Our research covers the comprehensive understanding of the physiological roles of various kinds of biocatalysts and receptors as well as the reaction mechanism and specificity of each enzymatic reaction. **1)** Chemical, biochemical and molecular biological studies on β -primeverosidase (EC 3.2.1.149), a diglycosidase deeply concerned with tea aroma formation. **2)** Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ -glutamyltranspeptidase and γ -glutamylcysteine synthetase. **3)** Design and synthesis of glycosylamidines as new glycosidase inhibitors and their application to affinity chromatography. **4)** X-Ray crystallographic analysis of pyruvate phosphate dikinase from maize. **5)** Directed evolutionary studies of *Pseudomonas* lipase. **6)** Molecular mechanism of the activation/inactivation process of plant hormones (brassinosteroids, gibberellins, cytokinins, etc.) by cytochrome P450. **7)** Molecular mechanism of plant resistance against disease infection specially interested in non-pathogenic *Fusarium* (NPF)-induced-resistance in sweet potato (*Ipomoea batatas* L.).

Research Activities (Year 2002)

Presentations

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

- 1)** Disaccharide-specific glycosidase: β -primeverosidase, Sakata K, 75th Annual Meeting, Jpn. Soc. Biochem, 14 -17 October, Kyoto, 2002, and 2 papers in the other meetings.
- 2)** Transition-state analog inhibitors of *E. coli* γ -glutamyltranspeptidase (2nd report), Tachi N, Hiratake J, Suzuki H, Kumagai H, Sakata K, 2002 Annual and 426th Meeting of Kansai Branch of Jpn. Soc. Biosci, Biotech, and Agrochem, 5-6, October, Nara, 2002, and one paper in other meetings.
- 3)** Glycosylamidine as potent and selective glycosidase

inhibitors: synthesis and applications. Hiratake J, 5th Hirschegg Winter School on Chemical Biology, Hirschegg, Austria, February 16 - 23, 2002, and **6 papers** in other meetings and symposia.

4) X-Ray crystallographic study on PPK from maize, Nakanishi T, Nakatsu T (RIKEN), Matsuoka M (Nagoya Univ), Kato H (RIKEN), Sakata K, 2002 Annual Meeting Jpn. Soc. Biosci, Biotech, and Agrochem, 24-27 March, Sendai, 2002.

5) Altering reaction specificity of lipase by evolutionary molecular engineering, Nakagawa Y, Fujii R, Hiratake J, Sogabe A (Toyobo Co., Ltd.), Sakata, K, 2002 Annual and

A Novel Disaccharide-Specific Glycosidase Family in Plants: β -Primeverosidase and Acuminosidase

Tea plants (*Camellia sinensis*) contain β -primeverosides with various aglycons as aroma precursors, and the tea leaf β -primeverosidase is deeply concerned with the floral aroma formation in oolong tea and black tea during tea manufacturing processes. We have succeeded in the purification and cloning of the β -primeverosidase [1]. Based on the amino acid sequence similarity, the β -primeverosidase was classified into a family 1 glycosyl hydrolase. The β -primeverosidase exhibited the selective hydrolysis of β -primeverosides to liberate a primeverose unit and aglycons without cleaving the inter-glycosidic linkage between Xyl and Glc (Fig. 1). The stereochemistry for hydrolysis by the enzyme revealed that the β -primeverosidase catalyzed the hydrolysis of glycosyl bond with retention of the anomeric configuration (Fig. 2). We have also succeeded in cDNA cloning of a furcatin hydrolase from *Viburnum furcatum* Blume (Fig. 1). The furcatin hydrolase was clustered with the β -primeverosidase in phylogenetic analysis of family 1 glycosidases, suggesting that disaccharide-specific glycosidases form a new subfamily in the family (Fig. 3).

1. Mizutani M, Nakanishi H, Ema J, Ma SJ, Noguchi E, Inohara-Ochiai M, Fukuchi-Mizutani M, Nakao M, Sakata K, *Plant Physiol.*, 130, 2164 (2002)

426th Meeting of Kansai Branch of Jpn. Soc. Biosci, Biotech, and Agrochem, 5-6 October, Nara, 2002.

6) Biochemical characterization of tomato CYP72B involved in brassinosteroid catabolism, Ohnishi T, Mizutani M, Ohta D (Osaka Pref. Univ), Nomura T (Teikyo Univ.), Yokota T (Teikyo Univ.), Sakata K, 2002 Annual Meeting, Jpn Soc. Biosci, Biotech, Agrochem, 24-27 March, Sendai, 2002 and **1 paper** in the same meeting.

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, A new combinatorial method to determine substrate specificities of glycosidases, Grant-in-Aid for Exploratory Research, 1 April 2001 - 31 March 2003.

Hiratake J, Bio- and organic chemical studies on glycosidases by using transition-state and substrate

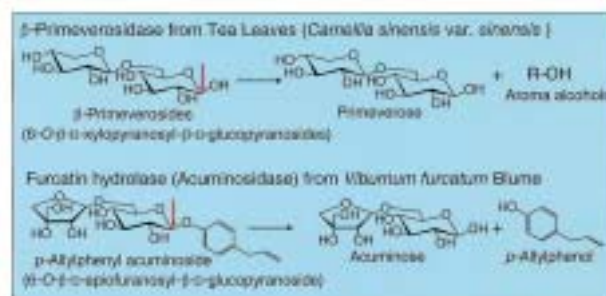


Fig. 1. Disaccharide-specific glycosidases in plants.

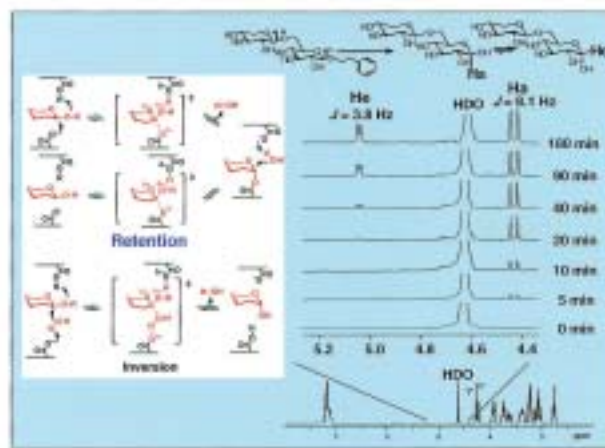


Fig. 2. Stereochemistry for hydrolysis.

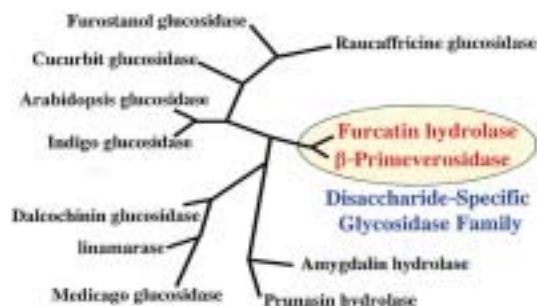


Fig. 3. Phylogenetic tree of family 1 glycosidases.

analogue inhibitors as a tool, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2004.

Mizutani M, Molecular mechanisms of the activation/inactivation of a plant hormone, Grant-in-Aid for Scientific Research Priority Areas (A), 1 April 2001 - 31 March 2003.

Shimizu B, Elucidation of synthetic pathway and physiological role of coumarins in plants, Grant-in-Aid for Scientific Research from Kyoto University, 1 April 2001 - 31 March 2001.

Award

Ma SJ, Mizutani M, Hiratake J, Hayashi K, Yagi K, Watanabe N, Sakata K, Award for excellence to authors publishing in Biosci, Biotech, Biochem, Substrate specificity of β -primeverosidase, a key enzyme in aroma formation during oolong tea and black tea manufacturing, Biosci. Biotechnol. Biochem. 65, 2719-2729 (2001), Jpn. Soc. Biosci, Biotech, and Agrochem. 24 March 2002.

Molecular Biofunction

- Molecular Microbial Science -

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Dr Daninel Darley	University of Marburg, Germany, 1 July 2002–12 July 2002

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 2002)

Presentations

Studies of the function of selenium in mouse brain, Kuwana E, Mihara H, Esaki N, 2002 Annual Meeting, Jpn. Soc. Biosci, Biotech, and Agrochem., 26 March.

Iron-sulfur cluster formation in *E.coli*: Properties of the IscS-IscU complex, Kato S, Mihara H, Kurihara T, Yoshimura T, Esaki N. 2002 Annual Meeting, Jpn. Soc. Biosci, Biotech, and Agrochem., 26 March.

Identification of the proteins involved in 2-chloroacrylic acid metabolism in *Burkholderia* sp., Kurata A, Kurihara T, Kamachi H, Esaki N, 2002 Annual Meeting, Jpn. Biochem. Soc., 16 October.

Properties of *N*-methyl-L-amino acid dehydrogenase of *Pseudomonas putida*, Kakutani R, Mihara H, Yasuda M, Ueda M, Esaki N, 2002 Annual Meeting, Jpn. Biochem. Soc., 17 October.

Grants

Esaki N, Structural biology and biosynthesis of sele-

nium-containing proteins, Grant-in-Aid for Scientific Research (B), 1 April 2001 - 31 March 2003.

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, Determination of whole genome sequence of psychrophilic bacteria, analysis of genes involved in their adaptation to cold environments, and exploitation of cold-active enzymes, Grant-in-Aid for Scientific Research (B) 1 April 2001 - 31 March 2003.

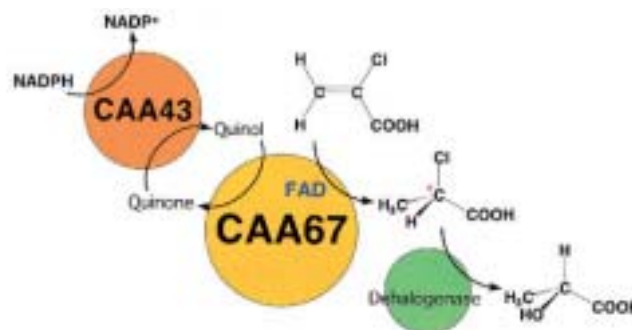
Mihara H, Analyses of *suf* gene cluster and Suf proteins involved in iron transport, Grant-in-Aid for Young Scientists B, 1 April 2001 - 31 March 2003.

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

A Novel Enzyme Catalyzing Asymmetric Reduction of Carbon-Carbon Double Bond

Asymmetric reduction of carbon-carbon double bonds is one of the most useful methods for production of chiral compounds. We have isolated a novel bacterium, *Burkholderia* sp. WS, catalyzing asymmetric reduction of 2-chloroacrylic acid to produce *S*-2-chloropropionic acid, which is the essential building block of aryloxyphenoxypropanoic acid, the herbicide skeleton most widely used for broadleaf crops such as cotton and soybean. In bacterium, 2-chloroacrylic acid is converted into *S*-2-chloropropionic acid, which is subsequently hydrolyzed to lactic acid by the action of 2-haloacid dehalogenase. The activity of 2-chloroacrylic acid reductase was induced when the bacterium was grown on 2-chloroacrylic acid as the carbon source, and we found that three proteins were inducibly synthesized in accordance with the induction of the reductase activity. One of them was supported to be 2-haloacid dehalogenase, and other two, named CAA67 and CAA43, were thought to participate

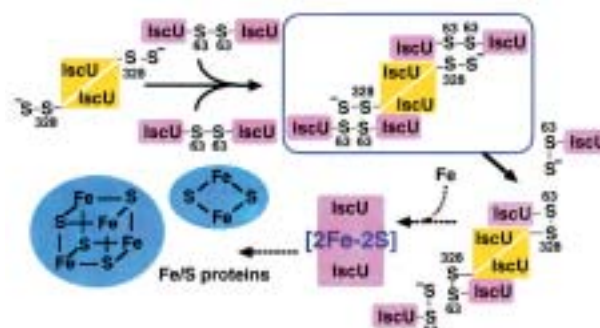


Scheme 1. Probable assimilation pathway of 2-chloroacrylic acid in *Burkholderia* sp. WS

in the reduction of 2-chloroacrylic acid. The genes coding for CAA67 and CAA43 were cloned and sequenced. The two genes constituted a gene cluster. CAA67 and CAA 43 showed sequence similarity to fumarate reductase and NAD(P)H: quinone oxidoreductase, respectively. CAA 67 probably catalyzes reduction of 2-chloroacrylic acid, and CAA43 most likely functions as a supplier of reducing power for CAA67.

Assembly of Iron-Sulfur Cluster in *Escherichia coli*

Iron-sulfur proteins are widely distributed in organisms and play essential roles in energy metabolism, DNA repair, transcriptional regulation, and biosynthesis of nucleotides and amino acids. Recent studies demonstrated that the assembly of their prosthetic groups, iron-sulfur clusters, is mediated by proteins encoded by the *isc* operon in prokaryotes and by their counterparts in eukaryotes. Among these proteins, IscS catalyzes the desulfurization of L-cysteine and cooperates with IscU in the biosynthesis of iron-sulfur clusters in *E. coli*. IscS and IscU form a covalent complex, and a sulfur atom derived from L-cysteine is transferred from IscS to IscU. We found that the disulfide bond is formed between Cys328 of IscS and Cys63 of IscU. We also found that Cys 63 of IscU is essential for the IscU-mediated



Scheme 2. Formation of iron-sulfur clusters

activation of IscS.

Based on the findings, we propose a mechanism for an early stage of iron-sulfur cluster assembly: the sulfur transfer from IscS to IscU is initiated by the attack of Cys63 of IscU on the S_γ atom of IscS-Cys328 that is bound to sulfane sulfur derived from L-cysteine.

for Young Scientists A, 1 April 2002 - 31 March 2004.

Yoshimura T, Construction of Enzymes with new functions by loop engineering, Seed Research Program of Biotechnology, Ministry of Agriculture, Forestry, Fisheries of Japan, 1 April 2000 - 31 March 2005.

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 -

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Scope of Research

Our research aims are to elucidate structure-function relationships of biological macromolecules, mainly proteins, by using X-ray diffraction method and other physicochemical methods. The following attempts have been mainly made in our laboratory for that purpose. (1) X-ray diffraction studies on protein structures in crystal and in solution are carried out by crystallographic and/or small-angle X-ray scattering techniques to elucidate structure-function relationships of proteins. (2) Molecular mechanism for myosin assembly is studied by proteolytic method, electron microscopy, and computer analysis of the amino acid sequence.

Research Activities (Year 2002)

Presentations

Structure-based analysis of functional sites of thermostable aspartase, Fujii T, Sakai H, Kawata Y (Tottori), Hata Y, XIX Congress and General Assembly of the International Union of Crystallography, 7 - 10 August.

Crystal structures of pokeweed lectins; Hayashida M, Fujii T, Ishiguro M (Kyusyu), Hata Y, Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 26 March; Annual Meeting, Prot. Sci. Soc. Jpn., 14 June, Kyushu Symp. on Struct. Funct. Prot. Enzy., 18 July, XIX Congress and General Assembly of the International Union of Crystallography, 12 - 15 August, Annual Meeting, Jpn. Biochem. Soc., 16 October, Annual Meeting, Crystallogr. Soc. Jpn., 11 December.

Detection of Change in Protein Quaternary Structure by Scattering Method: Observation of Degradation and Reconstitution of Chaperonin Proteins GroEL & GroES, Hiragi Y, Ichimura K (Dokkyo), Seki Y (Nagoya), Higurashi T (Osaka), Kawata Y (Tottori), Soda K

(Nagaoka), XII International Conference on Small-Angle Scattering, 25 - 29 August.

Structure of ADP dependent thermophilic bacteria *Pyrococcus horikoshii*, Kujime A (Tokushima), Hiragi Y, Tsuge H (Tokushima), Ichimura K (Dokkyo), Goda, S (Tokushima), Sakuraba H (Tokushima), Ohshima, T (Tokushima), Annual Meeting, Jpn Biochem. Soc., 14 - 17 October.

Role of electrostatic interactions in myosin filament formation, Akutagawa T, Hata Y, Ooi T and Katayama E (Tokyo), Annual Meeting, Bophys. Soc. Jpn., 4 November.

Grants

Fujii T, Elucidation of reaction mechanism of high-active-thermostable aspartase by crystallographic analyses of complexes, Grant-in-Aid for Encouragement of Young Scientists, 1 April 2000 - 31 March 2003.

Detection of Change in Protein Quaternary Structure by Scattering Method: Observation of Degradation and Reconstitution of Chaperonin Proteins GroEL & GroES

Although light scattering, CD, fluorescence and sedimentation have so far utilized monitoring the structural change of oligomeric proteins, no direct detection of the quaternary structure was possible by these methods. The Kratky plot of small-angle scattering intensities can assign the structure. State of the denatured entity is also estimable from the pair wise plots of forward scattering intensities and z-average radii of gyration.

1) On GroEL denaturation, peaks on the Kratky plots disappeared at the GdnHCl concentration of 0.8M. From the calculation based on the atomic co-ordinates, it was proved that the peaks originated in the quaternary structure of the tetradecameric oligomer. Pair wise plots of change in forward scattering intensities and z-average radii of gyration obtained from SAXS measurements indicate GroEL 14-mer directly denatured to unfolded coil without passing through the globular monomer in the present case.

2) Denaturation of GroES by GdnHCl showed that the quaternary structure was lost at 1.2M GdnHCl. Denatured coil structured GroES was completely reconstructed to heptameric native oligomer by diluting the GdnHCl judged by the coincidence of radius of gyration and profiles of Kratky plot and distance distribution function between original native structure and that of reconstituted one.

3) In the case of heat denaturation, GroES was denatured at 62 °C and also reconstructed, in the sense of structure, by lowering the temperature.

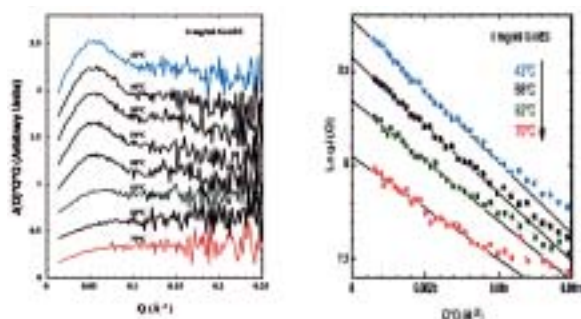


Figure 1. Heat dissociation/unfolding and refolding/reassociation of GroES. The solution condition is 0.5M GdnHCl with 20mM phosphate buffer (pH 7.0).

Role of electrostatic interactions in myosin filament formation

In myosin assembly into thick filaments, the myosin molecules are packed with axial staggers of 14.3 nm and 43 nm. In order to define how these staggers are caused between the rod segments of the adjacent molecules, energy calculation of electrostatic interaction between parallel two rod fragments, when the one fragment shifts along the other, was performed using the rod structure (α -helical coiled coil) and the amino acid sequence of the rod fragment. This amino acid sequence is highly repetitive by alternate clusters of positive and negative charge. Energy of the electrostatic interaction is based on the Debye-Huckel electrostatic potentials, and sum of these potentials is represented as difference of free energy between dimer formation and monomer state of the two fragments, according to procedure which was developed by Ooi. Obtained energy profile shows that a peak as the lowest free energy appears at shift of 14.3 nm. And also, a lower peak appears at shift of 43 nm. From these lower free energies, the most stable dimer is formed through these shifts, then the most stable thick filament would be formed through staggers of 14.3 nm and 43 nm. Consequently, it is strongly suggested that electrostatic interaction plays a crucial role for these staggers. This work is final achievement of Professor Dr. Tatsuo Ooi, Professor Emeritus of Kyoto University, who passed away on 25th September 2002.

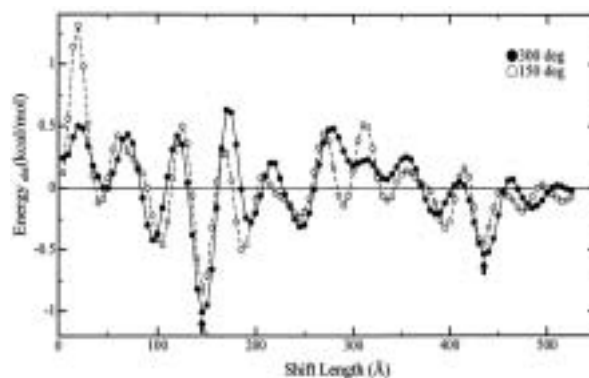


Figure 2. Electrostatic interaction between two parallel rod fragments when the one fragment shifts along the other. This fragment has ability to form paracrystal with a structural repeat of 43 nm. Interaction energy is caused by surface charge clusters of the fragments. Lower values of energy correspond to stronger electrostatic attractions.

Molecular Biology and Information

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Scope of Research

The major subjects are mechanisms involved in signal transduction and regulation of gene expression responsive to environmental stimuli, differentiation and development of plant organs, and plant-microbe interaction. As of December 2002, study is being concentrated on the roles of two-component response regulators and homeodomain proteins of higher plants in signal transduction and developmental processes.

Research Activities (Year 2002)

Presentations

The transcription factor-type response regulator ARR1 is involved in an early step of cytokinin signal transduction, Oka A, Aoyama T, Honma T, Sakai H, 2002 Ann Meeting of Jpn. Soc. Plant Physiol.: Symposium 'Phytohormone signal transduction for physiological functions', 28 - 30 March (Okayama).

Transcription factors ARR1 and ARR2 controlling cytokinin responses, Aoyama T, RIKEN Symposium 'Signal perception and transduction in higher plants', 26 April (Wako).

Isolation and analysis of direct target genes for the transcriptional regulation of ATHB-1, Muramoto T, Oka A, Tabata S, Lucchetti S, Morelli G, Ruberti I, Aoyama T; Initial step of root hair morphogenesis regulated by the transcription factor GLABRA2, Ohashi Y, Oka A, Pousada RR, Ruberti I, Morelli G, Aoyama T, 28 June - 2 July, XIII International Conference on Arabidopsis Research (Seville, Spain).

Grants

Oka A, Research project for network mutually controlling plant responses to environmental stimuli with morphogenesis: Hierarchy of transcriptional controls in plant signal transduction, Special Coordination Fund of the Ministry of Education, Culture, Sports, Science, and Technology of Japan, 1 April 1997 - 31 March 2003.

Aoyama T, Functional analysis of homeodomain proteins controlling the flexibility of plant morphogenesis, Grant from the Bio-oriented Technology Research Advancement Institution (BRAIN), 1 April 1998 - 31 March 2003.

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.

Sakai H, Molecular basis of cytokinin signalling in plant cells, Grant-in-Aid for Scientific Research on Priority Areas (A), 1 April 2002 - 31 March 2003.

The *Arabidopsis* response regulator ARR1 is a transcription factor for genes immediately responsive to cytokinins

Bacteria have devised phosphotransfer signalling mechanisms for eliciting a variety of adaptive responses to their environment. These mechanisms are collectively referred to as two-component regulatory systems. Each system generally consists of a sensor protein histidine kinase, which is anchored in the cell membrane, and a cytoplasmic response regulator, whose activity is modulated by the sensor. Most response regulators are transcription factors. We have recently presented the evidence for the existence of quite similar systems in higher plants, such as the signal transduction induced by the phytohormone cytokinin [1, 2]. The *Arabidopsis* CRE1 histidine kinase and its related proteins *AHK2* and *AHK3* perceive cytokinins in the environment and transduce a signal, presumably through the AHP bridge components that carry the histidine-containing phosphotransfer (HPT) domain, to the ARR1 response regulator that transcriptionally activates genes (e.g. *ARR6*) immediately responsive to cytokinins (Figure 1).

The *Arabidopsis* genome additionally codes for 10 ARR1-like response regulators, most of which also appear to be involved in cytokinin signalling. Besides, the *Arabidopsis* genome provides another type of 11 response regulators (e.g. *ARR6*) that are not transcription factors. They are quickly induced by cytokinins through ARR1 directly. Although ethylene and daylight signalling are also triggered by sensor histidine kinases (e.g. *ETR1* and *PHYB*), no corresponding response regulators have been identified. Therefore, the cytokinin signalling process may participate in cross-talk with signalling systems that respond to ethylene and daylight, through an intra-

cellular pool of several ARR1-like molecular species.

1. H. Sakai, T. Aoyama, and A. Oka, *Plant J.*, **24**, 703-711 (2000).
2. H. Sakai, T. Honma, T. Aoyama, S. Sato, T. Kato, S. Tabata, and A. Oka, *Science*, **294**, 1519-1521 (2001).

Entopically additive expression of *GLABRA2* alters the frequency and spacing of trichome initiation

During plant development, proliferated cells undergo morphological and physiological differentiation that allows specialized function. Among various cell types in plants, *Arabidopsis* trichomes have been used as a model to study plant cell differentiation. A trichome is a hair-like structure on the surface of a plant shoot, consisting of a single cell that develops in a series of cellular events, including endoreduplication, cell expansion and outgrowth, branching, and cell wall maturation. As trichomes are not essential for growth, many mutants defective in trichome development have been isolated. Most of these mutants are divided into two classes based on their phenotypes. The first class participates in the initiation of trichome development, e.g. *GLABRA1* (*GL1*) and *TRANSPARENT TESTA GLABRA1* (*TTG1*). Defects of this class change the initiation frequency or spacing of trichomes. The second class is related to trichome cell morphogenesis. Defects in this class result in the generation of aberrant trichomes.

GLABRA2 (*GL2*)/*ATHB-10* categorized in the second class encodes a homeodomain protein that belongs to the homeodomain-leucine zipper family. *GL2* is involved in not only trichome development, but also root hair and seedcoat development. We have here studied the role of *GL2* in trichome development [3]. A transgene consisting of a *GL2*-coding fragment preceded by the cauliflower mosaic virus 35S promoter (*35S::GL2*) does not complement *gl2-1* mutant defects. In the wild-type genetic background, *35S::GL2* causes *gl2*-mutant-like and scarcely viable phenotypes, suggesting that ectopic overexpression of *GL2* interrupts endogenous *GL2* function in trichome development, being toxic to plants. On the other hand, another *GL2* transgene containing the *GL2* promoter (*pGL2::GL2*) complements the *gl2-1* defects. Entopically additive expression of *GL2* by introduction of *pGL2::GL2* in the wild-type genetic background noticeable increases the number of trichomes and induces production of adjacent trichomes. In addition, *gl2-1/+* heterozygous leaves have fewer trichomes than *+/+* wild-type leaves. These results indicate that the amount of *GL2* in cells correlate with the frequency of trichome initiation, thereby being involved in determining trichome spacing.

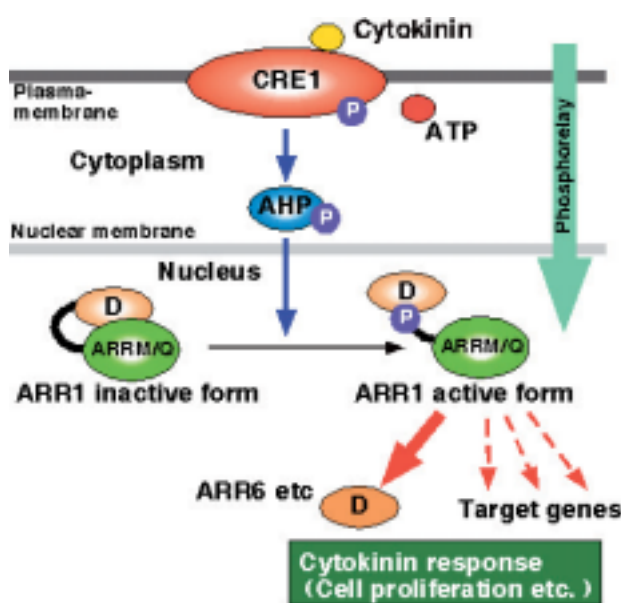


Figure 1. Model of cytokinin signal transduction.

3. Y. Ohashi, A. Oka, I. Ruberti, G. Morelli, and T. Aoyama, *Plant J.*, **29**, 359-369 (2002).

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The Institute for Genomic Research July 2001–August 2001

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 behaviors 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 2002)

Grants

Kanehisa M, Deciphering genetic and molecular networks by comparative genomics and systematic interaction experiments. Genome Frontier Project, MEXT.

Kanehisa M, Biological systems database 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.

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

Nakaya A, Extraction of correlated gene clusters by parallel data mining, Grant-in-Aid for Scientific Research on Priority Areas "Genome Information Science", MEXT.

KEGG Orthology : a 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 a new on-going project to identify and classify functional orthologs hierarchically 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).

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

New sequence motifs : intracellular transport system

In eukaryotic cells, macromolecules like proteins and lipids are transferred between organelles by the vesicular transport system, and specific recognitions on the transport pathway are mediated by SNARE superfamily proteins. We collected candidates of SNARE proteins from KEGG/GENES database, and classified them by the hierarchical clustering method (Fig. 3). As the result, SNARE proteins were found to form clusters depending on their subfamilies and intracellular localization sites, and a new sequence motif was found for every cluster.

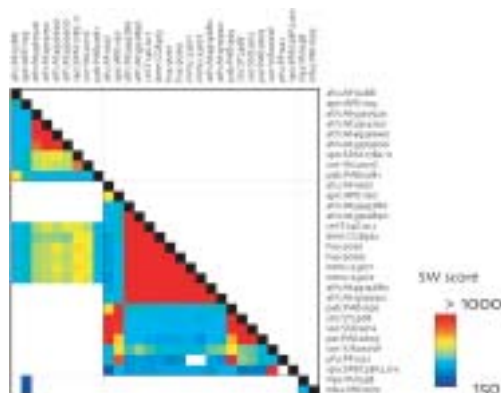


Fig. 1 All genes are clustered on the KEGG/SSDB scores.

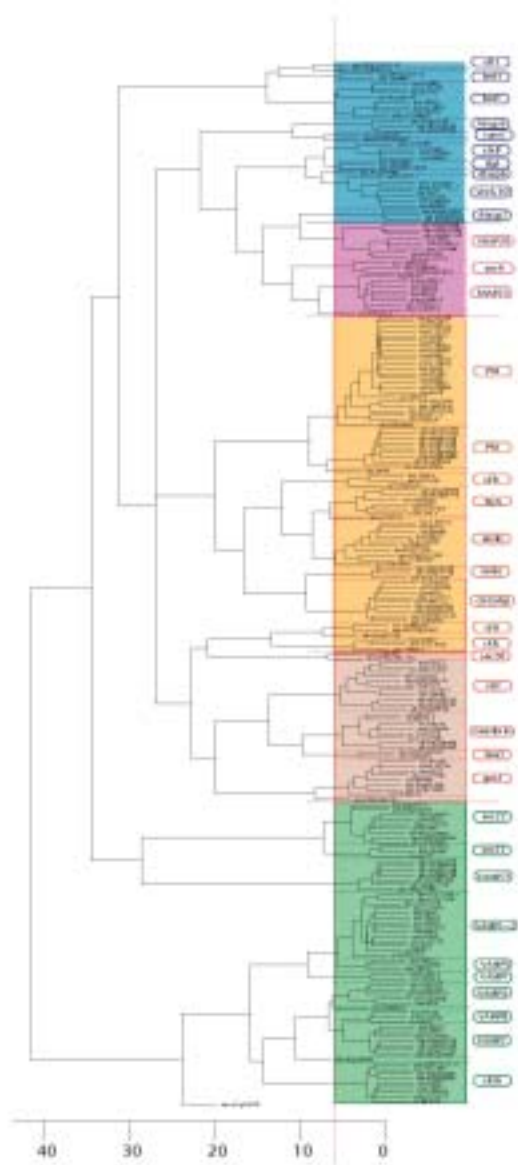


Fig. 3 SNARE proteins are clustered depending on their intracellular localization sites.

Bioinformatics Center

- Biological Information Network -

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



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Prof JIANG, Tao University of California, Riverside, 1 July 2002

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: data mining from chemical reaction data, protein structure prediction, motif extraction, inference of metabolic pathways and genetic networks, and analysis of two-dimensional electrophoresis gel images.

Research Activities (Year 2002)

Presentations

On the complexity of deriving position specific score matrices from examples, Akutsu T, Bannai H (U Tokyo), Miyano S, Ott S (U Tokyo), Annual Symp. Combinatorial Pattern Matching, 3 July.

Inferring a union of halfspaces from examples, Akutsu T, Ott S (U Tokyo), Int. Conf. Computing and Combinatorics, 15 August.

A gibbs sampling algorithm for numerical sequences: detection of subtle motifs from protein sequences and structures, Akutsu T, Annual Meeting of Korean Society for Bioinformatics, 15 November.

Point matching under non-uniform distortions and protein side chain packing based on an efficient maximum clique algorithm, K.C. Dukka Bahadur, Akutsu T, et al., Int. Conf. Genome Informatics, 18 December.

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.

Remote homology detection for proteins based on support vector machines

Recently, several methods were developed for remote homology detection for protein sequences using SVMs (support vector machines). We propose a new SVM based method (SVM-SW), which uses the SW algorithm as a kernel function (Fig. 1). Though we do not yet succeed to prove that the SW score is always a valid kernel, SVM-SW worked successfully in all cases we tested and was better than several existing methods.

1. H. Saigo et al., Comparison of SVM-based methods for remote homology detection, *Genome Informatics*, **13**, 396-397 (2002).

Point matching under non-uniform distortions and protein side chain packing based on an efficient maximum clique algorithm

We developed maximum clique-based algorithms for spot matching for two-dimensional gel electrophoresis images, protein structure alignment and protein side chain packing. Algorithms based on direct reductions to the maximum clique can find optimal solutions for instances of size (the number of points or residues) up to 50-150 using a standard PC. We also developed pre-processing techniques to reduce the sizes of graphs. Combined with some heuristics, many realistic instances can be solved approximately.

1. Dukka Bahadur K. C. et al., Point matching under non-uniform distortions and protein side chain packing based on an efficient maximum clique algorithm, *Genome Informatics*, **13**, 143-152 (2002).

On the complexity of deriving position specific score matrices from examples

PSSMs (Position-Specific Score Matrices) have been applied to various problems in Bioinformatics. We study the following problem: given positive examples (sequences) and negative examples (sequences), find a PSSM which correctly discriminates between positive and negative examples (Fig. 2). We proved that this problem is solved in polynomial time if the size of a PSSM is bounded by a constant. On the other hand, we proved that this problem is NP-hard if the size is not bounded. We obtained similar results on deriving mixture of PSSMs.

1. T. Akutsu et al., On the complexity of deriving position specific score matrices from examples, *Lecture Notes in Computer Science*, **2373**, 168-177 (2002).

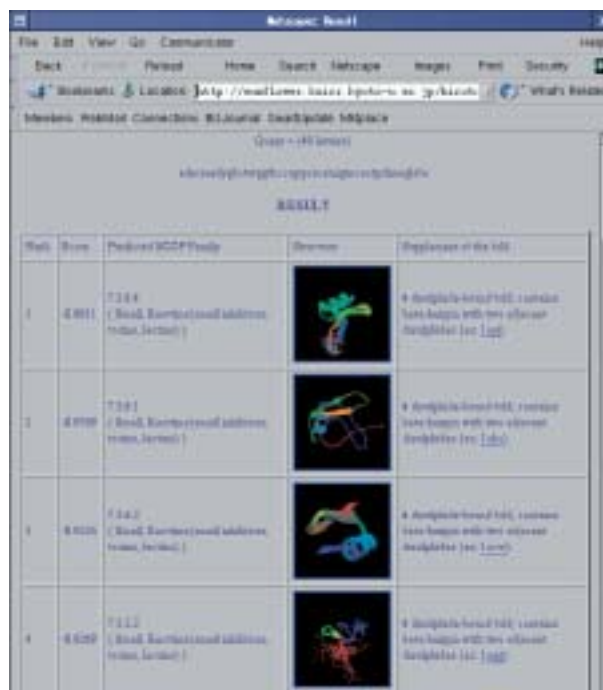


Figure 1. A system for remote homology detection of proteins.

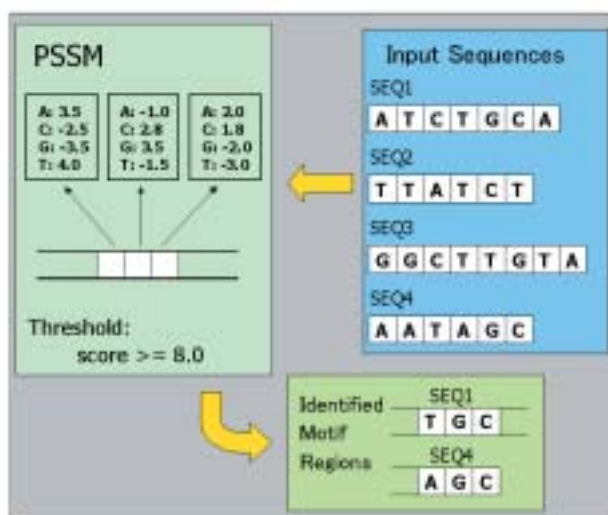


Figure 2. Motif detection using a position specific score matrix.

Bioinformatics Center

- Pathway Engineering -



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Scope of Research

This laboratory 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 2002)

Presentations

Estimation of genetic networks and functional structures between genes by using Bayesian networks and nonparametric regression, Imoto S, Goto T, Miyano S, Pacific Symposium on Biocomputing 2002, Hawaii, USA, Jan 3 - 7, 2002.

Inferring, modeling and simulating biopathway, Miyano S, Journee Ouvertes Biologie Informatique Mathematique 2002 (JOBIM 2002), St. Malo, France, 10 - 12 June, 2002.

Genomic Object Net in JAVA (Ver.1.0): a general platform for biopathway modeling and simulation, Miyano S, The Fourth Biopathway Consortium Meeting, Edmonton, Canada, 1 - 2 August, 2002.

Bayesian network and nonparametric heteroscedastic regression for nonlinear modeling of genetic network, Imoto S, Kim S, Goto T, Aburatani, S (Kyushu U), Tashiro K (Kyushu U), Kuhara S (Kyushu U), Miyano S, The First IEEE Computer Society Bioinformatics Conference, Stanford, USA, 15 - 17 August, 2002.

Inferring gene regulatory networks from time-ordered gene expression data using differential equations, de Hoon MJL, Imoto S, Miyano S, The 5th International Conference on Discovery Science, Luebeck, Germany, 24 - 26 November, 2002.

A string pattern regression algorithm and its application to pattern discovery in long intron, Bannai H, Inenaga S (Kyushu U), Shinohara A (Kyushu U), Takeda M (Kyushu U), Miyano S, The Thirteenth International Conference on Genome Informatics, Tokyo, Japan, 16 - 18 December, 2002.

Grants

Miyano S, Genome-Wide Analysis of Genes Related to Disease Susceptibility and Drug Responsiveness, Research for Future Programs by Japan Society for the Promotion of Science, 1 April 2000 - 31 March 2004.

Miyano S, Mathematical Foundations of Computational Knowledge Discovery from cDNA Microarray Data, Grant-in-Aid for Scientific Research (B)(1), 1 April 2000 - 31 March 2003.

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. Fig. 1 shows some aspects of data and computational topics towards understanding of biological systems. 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 Bayesian network and nonparametric heteroscedastic regression that can cope with variances in microarrays.

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 (Fig. 2). We also have developed a tool which transforms biopathway models in KEGG and BioCyc to the GON XML files. Especially, all metabolic pathway models in KEGG are now ready for re-modeling and simulation with GON (Fig. 3). This tool can also be extended to cope with another biopathway databases.

Systems biology has a chance to create a new paradigm for drug target selection by employing computational modeling of gene networks. As an application of these efforts, we have recently succeeded in discovering an antifungal medicine target gene by analyzing gene networks constructed with our methods from cDNA microarray gene expression profile data of *S. cerevisiae* based on gene disruptions and drug doses.

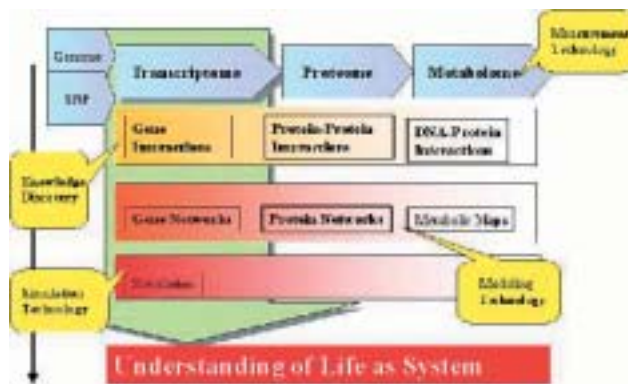


Fig. 1: Genome-wide data and computational issues towards understanding of life.

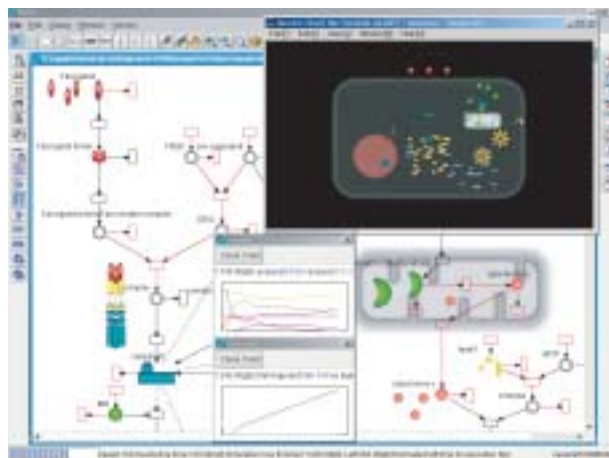


Fig. 2: Modeling and simulation of Fas ligand induced apoptosis pathway with Genomic Object Net.

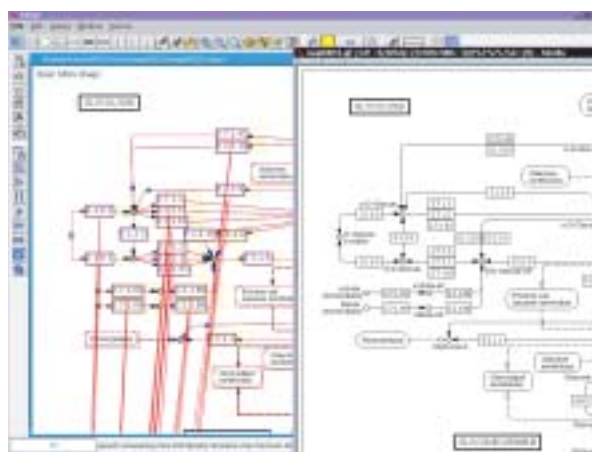


Fig. 3: A biopathway view of KEGG (right window) and its corresponding GON biopathway view (left window) that is simulatable with GON.

Contributed Chair

- Proteome Informatics (SGI Japan) -

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



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Scope of Research

With the advent of recently developed high-throughput experimental technologies, extremely large amounts of molecular biological data have been accumulated in these few years. With increasing the size of the data, both time- and space-efficient computational approaches have been strongly required to analyze the large-sized data sets. The primary objective of the laboratory is to establish and develop new computationally efficient methods and algorithms that allow us to better understand biologically important disciplines, such as rules, hypotheses, models and knowledge representations, from the vast amount of data of genomics and proteomics. The secondary objective is to implement the techniques developed by the laboratory as in softwares which will be used in molecular biology and related fields, such as (bio)chemistry, pharmacology and medical science. Research theme in the laboratory focuses on the issues related to proteins, with particular emphasis on protein-protein and protein-ligand interactions.

Research Activities (Year 2002)

Presentations

Dynamic Experimental Design Methodology Based on Query Learning and its Applications to Prediction of MHC Class I Binding Peptides, Abe N (IBM Watson Res. Center), Udaka K (Kyoto U), Mamitsuka H, Nakaseko Y (Kyoto U), Post-Genome Knowledge Discovery, Workshop on Protein Interactions and Clinical Data Analysis, Singapore, 28 May.

Iteratively Selecting Feature Subsets for Mining from High-Dimensional Databases, Mamitsuka H, Proceedings of the Sixth European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD02), Finland, 21 Aug.

Tree-width of chemical compounds in molecular biology

Building a method for measuring a quantitatively-significant similarity score between two arbitrary given compounds is an important issue in recent chemoinformatics and bioinformatics. If we obtain the similarity score within a relatively short time, it would be useful in a variety of both scientific and engineering applications related to chemistry and molecular biology. For tackling the issue, we deal with (the structure of) a given chemical compound as a 'molecular graph' and consider the usage of chemical and biological properties of the compound. As the first step of capturing the properties, we examined the 'tree-width', a measure indicating the complexity of a given graph, of chemical compounds particularly found in the context of molecular biology. The tree-width takes an integer in the range of 1 to $N-1$ for a graph with N nodes and increases as with increasing the complexity of the graph. More concretely, when a graph with N nodes is given, the tree-width is one if it is a tree, and the tree-width is $N-1$ if it is a complete graph. Figure 1 shows the schematic diagram representing the concept of the tree-width. The tree-width is a key concept in our study, because if the tree-width of a given set of graphs is bounded, it is known that for the set of graphs, a number of graph-related (NP-hard) problems, which are difficult to compute, can be solved within a relatively short (polynomial) computation time.

We obtained 9,712 chemical compounds from the LIGAND database [1] and computed the tree-width of each compound using an algorithm proposed by Matousek and Thomas in 1991 [2]. As shown in Figure 2, in all of the 9,712 cases except only one, the tree-width of a compound is an integer in the range of one to three, and the tree-width of the one exception is four. Experimental results show that the compounds whose tree-width is three or four are limited to some particular structures. For example, most of the compounds, whose tree-width is three, are Heme, which is shown in Figure 3. Figure 4 shows the structure of the compound whose tree-width is four. From the results, we conclude that the tree-width of a chemical compound in molecular biology is all relatively small, and we will be able to develop a time-efficient graph-theoretic algorithm for dealing with the compounds by using their biological and chemical properties.

1. Goto S, Okuno Y, Hattori M, Nishioka T and Kanehisa M: LIGAND: Database of Chemical Compounds and Reactions in Biological Pathways, *Nucleic Acids Res.*, **30**, 402-404 (2002).

2. Matousek J, Thomas R: Algorithms Finding Tree-Decompositions of Graphs, *J. Algorithms*, **12**(1), 1-22 (1991).

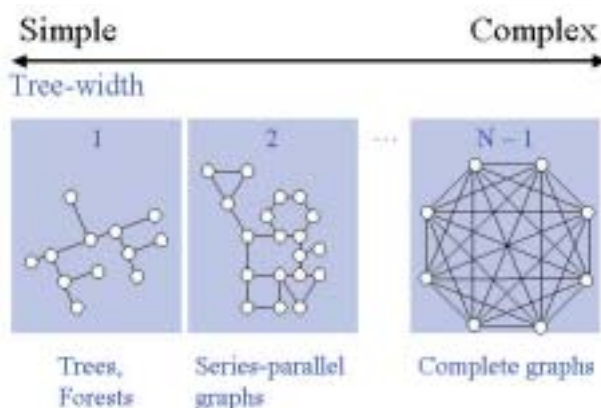


Figure 1. Tree-width: the complexity of a graph

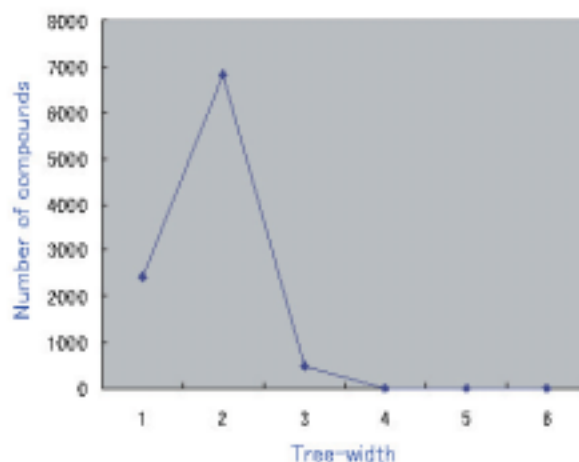


Figure 2. Distribution of tree-width of chemical compounds in LIGAND database

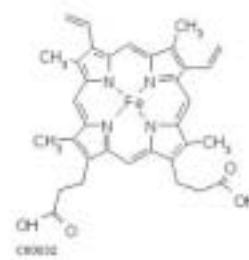


Figure 3. Heme (Tree-width: 3)

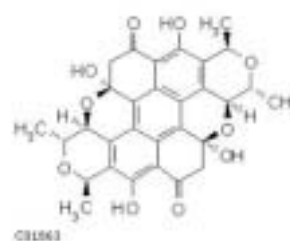


Figure 4. Xanthoaphin (Tree-width: 4)

Bioinformatics Center

- Bioinformatics Training Unit -

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Scope of Research

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

Research Activities (Year 2002)

Presentations

Pharmacoinformatics & Drug Design, Hiroyuki Toh, Symposium Roundtable: Science of Drug Design: Now and Future, The 122th Annual Meeting of the Pharmaceutical Society of Japan, Chiba, 27, March.

Three novel repetitive units of Reelin, Hisako Ichihara, Hisato Jingami, and Hiroyuki Toh, The 55th annual meeting of the Japan Society for Cell Biology, Yokohama, 21 May.

Molecular Phylogenetic Analysis of PCNA and the homologues. Hiroyuki Toh, Kazuya Osaka, and Yoshizumi Ishino, The 2nd Annual Meeting of the Protein Science Society of Japan, Nagoya, 13, June.

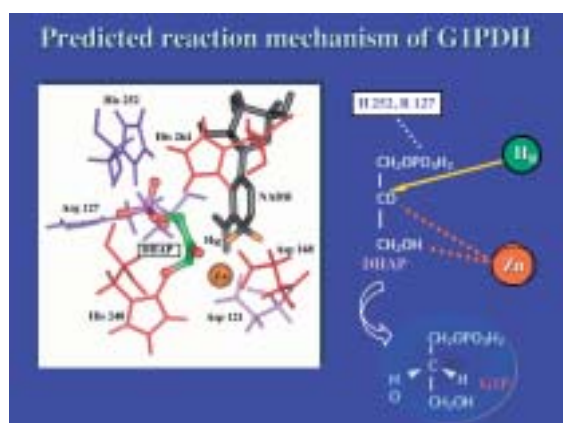
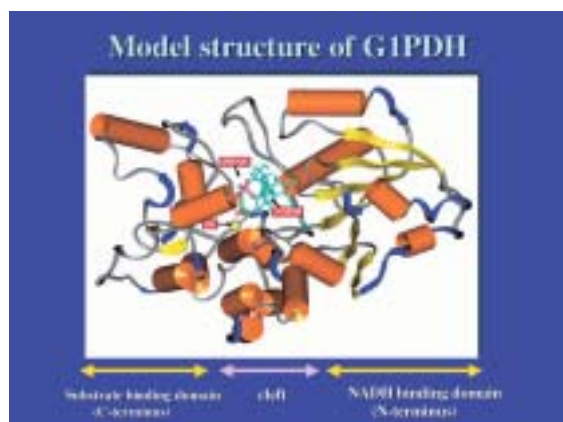
Inference of Genetic network from Expression Profile Data, Toh, H., and Horimoto, K., Workshop Bioinformatics orienting the analysis of inter-molecular interaction, The 2nd Annual Meeting of the Protein Science Society of Japan, Nagoya, 15, June.

Three novel repetitive units of Reelin, Hisako Ichihara, Hisato Jingami, and Hiroyuki Toh, The 3rd annual meeting of Chemo-Bio Informatics Society, Tokyo, 19, September.

The analysis of membrane stereochemistry with the homology modeling of sn-Glycerol-1-phosphate dehydrogenase, Hiromi Daiyasu, Hiroyuki Toh, Takaaki Hiroike, Yousuke Koga, The 3rd annual meeting of Chemo-Bio Informatics Society, Tokyo, 19, September.

An Analysis of Membrane Stereochemistry with Homology Modeling of sn-Glycerol-1-Phosphate Dehydrogenase

Different enantiomeric isomers, sn-glycerol-1-phosphate and sn-glycerol-3-phosphate, are used as the glycerophosphate backbones of phospholipids in the cellular membranes of Archaea and the remaining two kingdoms, respectively. In Archaea, sn-glycerol-1-phosphate dehydrogenase is involved in the generation of sn-glycerol-1-phosphate, while sn-glycerol-3-phosphate dehydrogenase synthesizes the enantiomer in Eukarya and Bacteria. The coordinates of sn-glycerol-3-phosphate dehydrogenase are available, al-



though neither the tertiary structure nor the reaction mechanism of sn-glycerol-1-phosphate dehydrogenase is known. Database searching revealed that the archaeal enzyme shows sequence similarity to glycerol dehydrogenase, dehydroquinase synthase, and alcohol dehydrogenase IV. The glycerol dehydrogenase, with coordinates that are available today, is closely related to the archaeal enzyme. Using the structure of glycerol dehydrogenase as the template, we built a model structure of the *Methanothermobacter thermautotrophicus* sn-glycerol-1-phosphate dehydrogenase, which could explain the chirality of the

product. Based on the model structure, we have determined the following: (1) The enzyme requires a Zn^{2+} ion for its activity. (2) The enzyme selectively uses the pro-R hydrogen of the NAD(P)H. (3) The putative active site and the reaction mechanism were predicted. (4) The archaeal enzyme does not share its evolutionary origin with sn-glycerol-3-phosphate dehydrogenase.

Ammonium-assimilating enzymes: physiological and phylogenic perspectives

Nitrogen-assimilating enzymes are important to produce organic nitrogen compounds. In the nitrogen-assimilating process, ammonium is converted into glutamate. There are two alternative pathways for the ammonium assimilation. One of them is composed of glutamate dehydrogenase (GDH), while the other consists of glutamine synthetase (GS) and glutamate synthase (GOGAT). Both pathways seem to be essential because our research clarified that many organisms had both pathways. The phylogenetic analyses of the three enzymes, GDH, GS, and GOGAT revealed that each enzyme had two or three paralogous subtypes. In many cases, however, each organism utilizes only one copy of subtypes. The adoption of the subtypes does not reflect the phylogenetic relationship.

Inokuchi R, Kuma K, Miyata T, and Okada M, *Physiologia Plantarum*, 116, 1-11, (2002).

Domain	Species	LBR		GR		LBRAT	
		I	II	I	II	I	II
Archaea	Comarchaeum			+	+		
						+	+
	Thermococcus					+	+
				+	+		
	Halobacterium sp.			+	+		
	Halobacterium salinarum			+	+		
	Halobacterium volcanium			+	+		
	Pyrococcus horikoshii			+	+		
	Thermoplasma acidophilum			+	+		
	Ignifluvis					+	+
Eubacteria	Aspergillus						
	Candida						
	Campylobacter			+	+	+	+
	Escherichia			+	+	+	+
	Staphylococcus						
	Thermotoga			+	+		
	Gram (+) Low-GC			+	+	+	+
	Gram (+) High-GC						
	Gram (+) alpha						
				+	+		
	Gram (-) beta			+	+		
	Gram (-) gamma						
				+	+		
	Gram (-) epsilon						
				+	+		
Eukaryotes	Animal			+	+		
	Fungi			+	+		
	Plant			+	+		

Nuclear Science Research Facility

- Particle and Photon Beams -

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Dr Evgeniy I. Antokhin
Dr Georg P.A. Berg

JINR, Dubna, Russia, February 7–8, August 20–26, 2002
POSTEC, Pohang, Korea, March 3–10, October 27–November 2, 2002
CERN, Geneva, Switzerland, April 26, 2002
BESSY, Berlin, Germany, April 30, 2002
BINP, Novosibirsk, Russia, June 21, 2002
KVI, Groningen, Netherland, December 3, 2002

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 2002)

Presentations

Ion beam cooling at Laser-equipped Storage and Cooler Ring, LSR, Noda A, Fadil H, Shirai T, Grieser M, Yamada S and Noda K., Annual Meeting Phys. Soc. Jpn., 24 March, 2002.

Design of Ion Cooler Ring, LSR at ICR, Kyoto University, Shirai T, Fadil H, Tongu H, Noda A et al., Annual Meeting Phys. Soc. Jpn., 24 March, 2002, The 8th European Particle Accelerator Conference, 6 June, 2002.

Electron Cooling of Ion Beams with Large Energy spread, Fadil H, Shirai T, Noda A, Grieser M et al., Annual Meeting Phys. Soc. Jpn., 24 March, 2002, The 8th European Particle Accelerator Conference, 5 June, 2002.

Ion production with a high-power short-pulse laser for application to Cancer Therapy, Noda A, Iwashita Y, Nakamura S, Shirai T, Tongu H et al., The 8th European Particle Accelerator Conference, 3 June, 2002, Ion production by focusing a high-power laser on a thin foil and its application, Nakamura S, Tongu H, Shirai T, Iwashita Y, Noda A, Daido H et al., Annual Meeting Phys. Soc. Jpn., 27 March, 2002.

Pulse stretcher of electron beam with use of the third integer

resonance and RFKO method, Sugimura T, Morita A, Tongu H, Shirai T, Iwashita Y and Noda A, Annual Meeting Phys. Soc. Jpn., 27 March, 2002, Pulse stretcher operation of the electron storage ring, KSR, Noda A, Fujimoto S, Iwashita Y, Shirai T, Tongu H, Morita A and Sugimura T, The 8th European Particle Accelerator Conf., 5 June, 2002.

Laser Ion Production as the Injector for Cancer Therapy Synchrotron, Noda A, Iwashita Y, Nakamura S, Shirai T et al., The 21st International Linac Conf., 22 August, 2002

Grants

Noda A, Beam Accumulation and Cooler Ring, Advanced Compact Accelerator Research, April 2002 - March 2003.

Iwashita Y, Super Strong Permanent Magnet for Final Focus Lens in Linear Collider, Grant-in-Aid for Scientific Research, (A) (1), April 2002 - March 2003.

Iwashita Y, High gradient acceleration with standing-wave structure for linear collider, KEK joint research and development program, April 2002 - March 2003.

Ion Production with High-Power Short-Pulse Laser

For the purpose of downsizing the scale and cost of the accelerator dedicated for cancer therapy, ion beams produced by focusing a high-power (100TW) short-pulse (20fs) laser on a solid thin film has been studied as a candidate for the injection beam into a pulse synchrotron. As such ion beams have wide energy spread, reduction of the energy spread with use of phase rotation as illustrated in Fig. 1, has been studied. The ion beams are accelerated or decelerated by the phase locked RF electric field to the pulse laser according to their arrival time at the RF cavity. With this scheme, energy spread is expected to be reduced from $\pm 5\%$ to $\pm 1\%$.

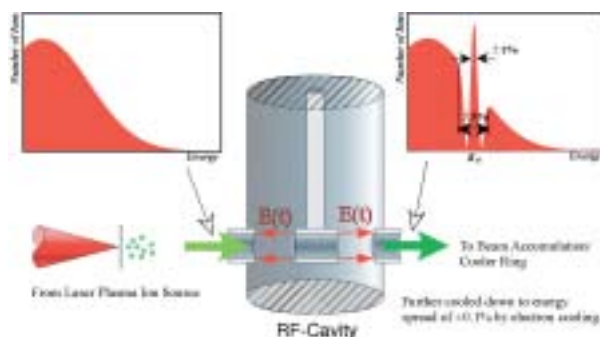


Figure 1 Scheme of phase rotation by RF electric field phase locked to the pulse laser.

Preliminary experimental results of laser ion production has been obtained using a pulse laser with several TW pulse peak power with duration of ~ 50 fs. In Fig. 2, the angular distributions of produced ions by the laser from thin foil targets of Ti(20 μ m) and CH(100 μ m). In this condition, the suppression of the pre-pulse is not sufficient and target-normal forward peak is not observed. Ions up to the energy of 600 keV are detected by CR39 plates.

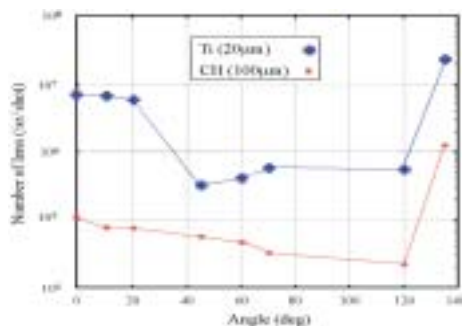


Figure 2 Angular distribution of produced ion number.

Electron Cooling of Hot Ion Beam

Electron cooling has so far been believed to be efficient only for rather cool beam [1] and is applied to cool down it to much



Figure 3 Scheme of electron cooling of hot ion beam with use of induction accelerator.

lower temperature. Stochastic cooling has been utilized to cool down hot ion beams as anti-protons produced from solid target. Stochastic cooling, however, needs longer cooling time for higher number of particles. In order to cope with this situation, a scheme to combine electron cooling with the acceleration by an induction accelerator is proposed [2] and has been tested with use of ion storage and cooler ring, TSR at Max-Planck-Institute für Kern Physik, Heidelberg, Germany[3].

As shown in Fig. 3, the electron cooling force is effective only in the region of the momentum spread of 0.1% (corresponds to energy spread of $\pm 0.1\%$). Our basic idea is to sweep the ion energy through this efficient cooling region by acceleration with induction accelerator. In Fig. 4, the needed time at TSR to shift the ion beam with the momentum -1% different from the central one to the center (0%) are shown for various induction voltages. It is known from the figure that the needed time to cool the beam -1% lower than the central momentum is factor 4 reduced from 2.8 s to 0.6 s by application of 0.4 V for the induction acceleration (maximum value attainable at TSR).

As the alternative of this method, the scheme to sweep the electron energy throughout the region of the ion beam energy spread by changing the high voltage to accelerate the electron is also tested at TSR. With this scheme cooling times for 1% momentum difference are measured to be 0.35 sec, 0.5 sec and 0.8 sec for beams with the horizontal size (FWHM) of 0.8 mm, 8 mm and 16 mm, respectively. Both methods are comparable and detailed studies are needed in connection with transverse beam size, which will be performed at LSR now under construction at NSRF, ICR, Kyoto University.

1. Möhl D, Proc. of ECOOL84, KfK 3846, 293 (1984)
2. Noda A et al., Beam Science and Technology, **6**, 21 (2001)
3. Fadil H et al., to be submitted to Nucl. Instr. and Meth.

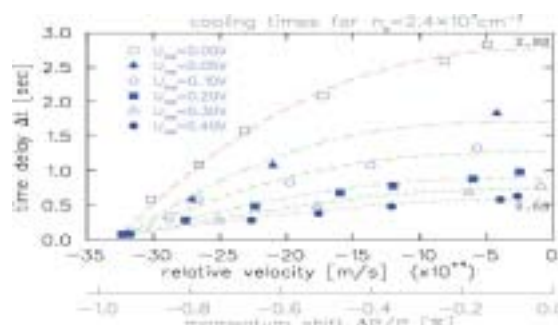


Figure 4 Cooling time for various induction voltage.

Nuclear Science Research Facility

- Beams and Fundamental Reaction -

<http://carrack.kuicr.kyoto-u.ac.jp>



Assoc Prof
MATSUKI, Seishi
(D Sc)



PD (JSPS)
HASEYAMA, Tomohito
(D Sc)

Researcher

TADA, Masaru (D Sc)

Students

KOMINATO, Kentaro (D4)

SHIBATA, Masahiro (D4)

Scope of Research

Atoms, nuclei, and dark matter particles in the Universe are studied with quantum electronic methods: Current research subjects are 1) search for a cosmological dark-matter candidate particle, axion, in the Universe with the Rydberg-atom cavity detector, 2) highly excited Rydberg atoms in an electric field and their applications to fundamental physics research, and 3) nuclear magnetism in 3-5 semiconductors with laser-assisted Overhauser process and optical pumping.

Research Activities (Year 2002)

Presentations

Selective pulsed-field ionization in highly excited Rydberg atoms (Experiment), Shibata M, Tada M, Kishimoto Y, Kominato K, Ooishi C, Yamada S, Saida T, Haseyama T, Funahashi H, Yamamoto K, and Matsuki S, Spring Meeting, Phys. Soc. Jpn., Kusatsu Shiga, 26 March.

Selective pulsed-field ionization in highly excited Rydberg atoms (Theory), Kishimoto Y, Tada M, Shibata M, Kominato K, Ooishi C, Yamada S, Saida T, Haseyama T, Funahashi H, Yamamoto K, and Matsuki S, Spring Meeting, Phys. Soc. Jpn., Kusatsu Shiga, 26 March.

Fourth-order dependence of the Stark shift on the electric field in highly excited Rydberg atoms, Haseyama T, Tada M, Kishimoto Y, Kominato K, Shibata M, Ooishi C, Yamada S, Saida T, Funahashi H, Yamamoto K, and Matsuki S, Spring Meeting, Phys. Soc. Jpn., Kusatsu Shiga, 26 March.

Review of axion searches, Matsuki S, First Sendai International Conference on Neutrino Science, Sendai, Japan, Sendai, 16 March.

Grants

Matsuki S, Search for Dark Matter Axions, Grant-in-Aid for Specially Promoted Research(2), 1 April 1997 - 31 March 2003.

Manipulating ionization path in a Stark map: stringent schemes to selectively field-ionize highly-excited Rydberg atoms

Rydberg atoms have been widely utilized for fundamental physics research [1,2]. Highly excited Rydberg states with the principal quantum number n larger than 80, however, have not yet been utilized in detail, partly because it is more difficult to detect selectively a particular state. It is important to develop a sensitive, selective ionization method for such highly-excited Rydberg atoms for further applications such as to long wavelength microwave detections. We investigated systematically the characteristics of the pulsed field ionization in the highly excited Rydberg states[3]. It was found that in these highly excited Rydberg states, the field ionization proceeds in two ways, that is, via 1) tunneling, and 2) autoionization-like processes. Indeed field ionization spectrum shows, in general, two peaks which are due to the two processes mentioned above. Lower peak is due to the process (2), while the higher peak corresponds to the process (1).

Along with these investigations, we have developed new stringent schemes to selectively ionize highly excited Rydberg atoms by manipulating the ionization path in a Stark map[4]: Low angular momentum states such as s and p states in Rb which are situated below and above the adjacent manifold, respectively, for example, are firstly chosen as initial states of interests. The s (p) state is then moved adiabatically to the lowermost (uppermost) state in the adjacent manifold by applying the slowly rising (low slew-rate) pulsed electric field, thereby transferring adiabatically the first avoided-crossing. Then the lowermost state is driven to higher electric field, thus causing ionization with a pulsed electric field in high slew-rate regime.

Manipulating schemes and resulting ionization spectra are shown in Fig. 1 together with the relevant Stark map and ionization paths. Related pulse profile is also shown in the figure. In order to make the selectivity more stringent further, applied pulsed field is modified as to have a three-step profile[4]. The spectrum observed with such a scheme clearly shows that the selection between the s and p states ionization-signals is quite stringent and much more improved than the previous one-step method[4].

These schemes can be applied to the quite sensitive microwave detection at the wavelength region of longer than 10 cm. One of such applications is to the detection of dark matter axions in microwave cavities[2,5]. Also the method may be applied to the detection of fundamental forces such as Casimir force.

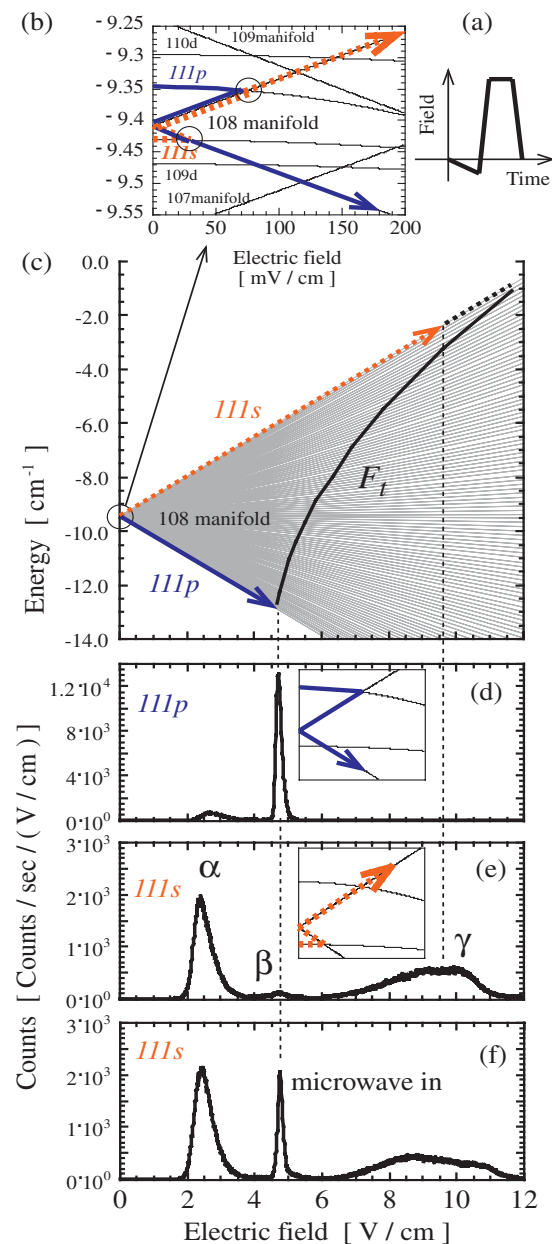


Fig.1 Stark energy diagram near the $n=108$ manifold and field ionization spectra of the $111p$ and $111s$ states with a pulsed field ionization scheme. a) pulse profile used, b) enlarged Stark map at low electric field region, c) Stark map near the 108 manifold, and ionization paths manipulated with the present schemes, d) ionization spectrum of $111p$ state, e) the same of $111s$ state, f) ionization spectrum of $111s$ state with microwave in, frequency of which corresponds to the transition frequency between the $111s$ and $111p$ states.

1. T. M. Gallagher, *Rydberg atoms* (Cambridge University Press, Cambridge, 1994).
2. I. Ogawa, S. Matsuki and K. Yamamoto, *Phys. Rev. D* **53** (1996) R1740, and references cited therein.
3. Y. Kishimoto et al., *Phys. Lett. A* **303** (2002) 279.
4. M. Tada, et al., *Phys. Lett. A* **303** (2002) 285.
5. K. Yamamoto et al., *Proc. Int. Conf. on Dark Matter in Astro- and Particle Physics*, Heidelberg, 2000 (Springer-Verlag, Heidelberg, 2001) p638.

LABORATORIES OF VISITING PROFESSORS

Solid State Chemistry - Structure Analysis -



Vis Prof
KANNO, Ryoji
(D Sc)

Professor

KANNO, Ryoji (D Sc)
Interdisciplinary Graduate School of Science and Engineering
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Lecture at *ICR*

Solid State Ionics



Vis Assoc Prof
MITANI, Seiji
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Associate Professor

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Magnetic Materials Laboratory
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Lecture at *ICR*

Tunneling Magnetoresistance in Granular Thin Films

Fundamental Material Properties - Composite Material Properties -



Vis Prof
YAMAMOTO, Yasushi
(D Eng)

Professor

YAMAMOTO, Yasushi (D Eng)
(ex-position) Director, Technological Strategy and Planning
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Lectures at ICR

Silicon Chemistry and Its Industrial Development
Silicone Resin and Its Application: (1) Organosilane Compounds and Silicone Oil
Silicone Resin and Its Application: (2) Silicone Elastomer and Modified Silicone
Development of Functional Silicon Materials: (1) Synthesis of Silicon
Dendrimers and their Functionality
Development of Functional Silicon Materials: (2) Electronic and Optical Materials



Vis Assoc Prof
SAITO, Hiromu
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Associate Professor

SAITO, Hiromu (D Eng)
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Lectures at ICR

Structure Control of Polymer Materials by Using Supercritical Fluid
Light Scattering Techniques for Characterization of Polymer Morphology
Molecular Motion and Deformation of Polymers

Synthetic Organic Chemistry - Synthetic Theory -



Vis Prof
NAKA, Takehiko
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Professor

NAKA, Takehiko (D Pharm Sc)
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Lectures at ICR

Research and Development of a Novel Antihypertensive Agent: Nonpeptide
Angiotensin II Receptor Antagonist, Candesartan Cilexetil



Vis Assoc Prof
SUGIHARA, Takumichi
(D Pharm Sc)

Associate Professor

SUGIHARA, Takumichi (D Pharm Sc)
Faculty of Pharmaceutical Sciences
Tokushima Bunri University
(Yamashiro-cho, Tokushima 770-8514)

Lecture at ICR

Relationship of Reactivity, Structure, and Ligand Effect in Cobalt Carbonyl Complexes



PERSONAL

Awards

TAMAO, Kohei

The 42nd Toray Science & Technology Prize (Toray Science Foundation)

"Organometallic Chemistry directed toward Organic Synthesis and Materials Science"

For the wide-ranging creative studies in organometallic chemistry, represented by the nickel-catalyzed cross-coupling reaction, the hydrogen peroxide oxidation of the silicon-carbon bond, and the development of silole-containing pi-conjugated systems and their application to the EL devices as efficient electron-transporting materials.

March 14, 2002

The award was established in 1960 to recognize distinguished contributions to the field of science and technology through innovative work of a great impact and, by such example, to stimulate the creativity of others. The award will be presented every year to two distinguished scientists. Among the first award recipients, we can see the name of Prof. Ichiro Sakurada, the former professor in our institute known as the innovator of the synthetic fiber Vinyon.

Frederic Stanley Kipping Award in Silicon Chemistry (The American Chemical Society)

"Distinguished Contributions to Organosilicon Chemistry"

For the wide-ranging creative studies in organosilicon chemistry, represented by the hydrogen peroxide oxidation of the silicon-carbon bond, the silole-containing pi-conjugated systems, and the functionalized silyl anions.

April 9, 2002



copyright, James Tkatch

The award was established in 1960 by Dow Corning Corporation to commemorate the achievements of Prof. Fredric Stanley Kipping, to recognize distinguished contributions to the field of silicon chemistry and, by such example, to stimulate the creativity of others. The award will be presented biennially. Prof. Tamao is the fourth Japanese recipient among the 28 recipients in the world.

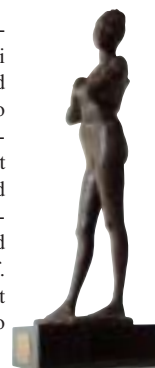
The Asahi Prize (Asahi Culture Foundation)

"Development of Innovative Organometallic Reactions"

For the wide-ranging creative studies in organometallic chemistry, represented by the nickel-catalyzed cross-coupling reaction, the hydrogen peroxide oxidation of the silicon-carbon bond known as the Tamao oxidation, and the development of silole-containing pi-conjugated systems and their application to the EL devices as efficient electron-transporting materials.

January 31, 2003

The award was established in 1929 by the Asahi Shimbun Co., to be presented to a person or a group who has made distinguished contributions to the development of the Japanese culture and society by producing prominent achievements in the field of art and science. Prof. Tamao is the first recipient among chemists in Kyoto University.



KOMATSU, Koichi

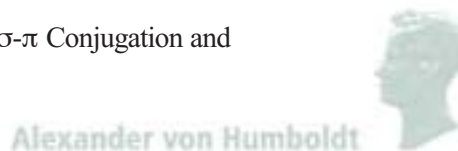


Humboldt Research Award (Alexander von Humboldt Foundation)

"Creation of Novel π -Electronic Systems Having σ - π Conjugation and Three-Dimensional π Conjugation"

Awarded for the achievements in the field of structural organic chemistry, particularly for (1) the development of the application of σ - π conjugation to control the electronic state of cyclic π -conjugated systems, which led to the first synthesis of superstable carbocations, the first isolation and structural determination of radical-cations of benzene, cyclooctatetraene, and polycyclic aromatic hydrocarbons, the first observation of silatropylium ions, and so forth, and (2) the discovery of the effectiveness of solid-state mechanochemical reaction in the first selective synthesis and structural determination of fullerene dimer C_{120} as well as trimer C_{180} .

November 11, 2002



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 150 most prominent researchers world-wide every year in all academic fields covering from natural science to the humanities.

KITANO, Tsuyoshi



The ICR Award for Students

"Exploration into the selectivity of ligands with coordinating nitrogen atoms of controlled distance first-series transition metal and Cd ions"

ICR

6 December 2002

YAMAGUCHI, Shigehiro



The Chemical Society of Japan Award for Distinguished Young Chemists

"Creation of Functional π -Electron Systems Containing Group 13, 14, and 15 Elements"

The Chemical Society of Japan

29 March 2002

AZUMA, Masaki



JSPM Award for Innovative Research

"Search for new transition metal oxides and single crystal growth by means of high pressure synthesis"

27 May 2002

TSUBAKI, Kazunori



The ICR Award for Young Scientists

"Molecular Recognition using Phenolphthalein Derivatives"

ICR

6 December 2002

KANAYA, Toshiji



SFSTJ Award

"Hierarchic Structure of Polymer Gels"

The Society of Fiber Science and Technology, Japan

22 May 2002

Paper Awards

SASAMORI, Takahiro; TAKEDA, Nobuhiro; TOKITOH, Norihiro

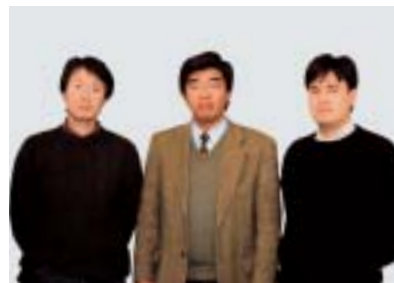
The Best Article of the Month

Bulletin of the Chemical Society of Japan, **75**, 661-675 (2002)

"Syntheses, Structures and Properties of Kinetically Stabilized Distibenes and Dibismuthenes, Novel Doubly Bonded Systems between Heavier Group 15 Elements"

The Chemical Society of Japan

25 September 2002



MA, Seung-Jin; MIZUTANI, Masaharu; HIRATAKE, Jun; HAYASHI, Kentaro; YAGI, Kensuke; WATANABE, Naoharu; SAKATA, Kanzo

Award for Excellence to Authors Publishing in 2001

Bioscience, Biotechnology, and Biochemistry, **65**, 2719-2729 (2001)

"Substrate Specificity of β -Primeverosidase, A Key Enzyme in Aroma Formation during Oolong Tea and Black Tea Manufacturing"

Japan Society for Bioscience, Biotechnology, and Agrochemistry

24 March 2002



Poster Awards

MIYAKE, Kousaku



Poster Award

17th International Colloquium on Magnetic Films and Surfaces (ICMFS 2002)

"Magnetic Domain Wall in a Nano-Contact between Two NiFe Wires"

7 March 2002

EJAZ, Muhammad



Best Poster Award

Macro Group UK, International Conference on Polymer Synthesis

"Fabrication of Patterned High-Density Polymer Graft Surfaces by Surface-Initiated Living Radical Polymerization"

Macro Group UK

1 August 2002

MASUDA, Kenji



Award for the Outstanding Paper

The Society of Polymer Science, Japan

30 May 2002

MURATA, Michihisa



Best Poster Award

16th Symposium on Fundamental Organic Chemistry

"Structure and Properties of an Open-Cage Fullerene Derivative Having a Sulfur Atom on the Orifice"

The Committee of 16th Symposium on Fundamental Organic Chemistry

5 October 2002

SHIRASAKA, Toshiaki



Symposium Poster Award

49th Symposium on Organometallic Chemistry, Japan

"Dibenzoborole-Based π -Electron Systems: Synthesis, Photophysics, and Sensing Ability for Fluoride Ion"

Kinki Chemical Society

13 September 2002

SHINOHARA, Akihiro



Symposium Poster Award

7th Symposium of the Society of Silicon Chemistry, Japan

"Synthesis and Properties of Kinetically Stabilized 1-Silanaphthalene"

The Society of Silicon Chemistry, Japan

25 November 2002

MORIKAWA, Hiroshi



Best Poster Award

"Effective Synthesis of Chiral Origo-Naphthalene Derivatives"

The Pharmaceutical Society of Japan (Kinki) and the Society of Synthetic Organic Chemistry, Japan (Kansai)

10 December 2002

YAMANAKA, Rio



Best Presentation Award

The 6th Japanese Symposium on the Chemistry of Biocatalysis

"Light-mediated Regulation of Asymmetric Reduction of Ketones"

Group Biocatalyst Chemistry Japan

12 December 2002

HIRANO, Toshiko



Best Poster Presentation Award

20th Joint Symposium between the Japan Society for Analytical Chemistry, 69th Symposium on Organic Micro-analysis and the Society of Instrument and Control Engineers, 59th Symposium on the Amount Measurement of Dynamics

"Analysis of Carbon, Hydrogen, and Nitrogen Contents in Silicon-Containing Compounds Using a YANACO CHN-CORDER MT-5"

The Association of Organic Micro-analysis

10 May 2002

TAKEHASHI, Masanori



Asia A Prize

The 18th International Congress of Clinical Chemistry and Laboratory Medicine

"Dinucleotide Repeats in Monoamine Oxidase A Gene Associated with Alzheimer's Disease and Lewy Body Variant"

The Organizing Committee of the 18th International Congress of Clinical Chemistry and Laboratory Medicine

23 October 2002

Obituary

Professor Emeritus

Dr. Tatsuo Ooi (1924 - 2002)



Professor Dr. Tatsuo Ooi, Professor Emeritus of Kyoto University passed away on September 25, 2002 in Kyoto.

Dr. Ooi was born on September 16, 1924 in Nagano. He entered the Department of Physics, Faculty of Science, Nagoya Imperial University in 1944 and was moved up to the Graduate School of Science, Nagoya Imperial University in 1947. After the graduation, he was appointed to an Instructor in the Department of Physics, Nagoya University in 1953, promoted to an Associate Professor in 1961, and got a Ph. D. (Doctor of Science) from Nagaya University in that year. He was promoted to a full Professor of the Institute for Chemical Research, Kyoto University in 1968 to direct the Laboratory of Physical Chemistry of Enzymes (presently the Laboratory of Biopolymer Structure, Division of Molecular Biology and Information I). From 1985 to 1987, he held concurrently a Professor of a newly founded laboratory, the Laboratory of Molecular Design of Physiological Functions (presently the Laboratory of Bioknowledge Systems, Bioinformatics Center). He did a lot of works in biophysical researches on structures of biological macromolecules such as proteins and DNAs and in computational analyses of DNA sequences. He also did his best to introduce an electronic computer to the Institute and served as the first head of the Central Computer Facility in the Institute. He retired from Kyoto University in 1988, honored with the title of Professor Emeritus of Kyoto University. After the retirement, he moved to the Faculty of Home Economics, Kyoto Women's University as a full Professor in 1988. From 1993 to 1996, he served as the chief librarian in the University. He retired from Kyoto Women's University in 1998.

Dr. Ooi's research field was concerned with biophysics. He contributed largely to the development of biophysics by producing lots of achievements in biophysical

researches, especially in theoretical and experimental studies on structures of biological macromolecules such as proteins and DNAs. One of his superior works was the development of the two-dimensional distance map, so-called "Ooi map", which has been used to visualize three-dimensional structures of proteins. He also exerted himself to make the DNA database and to develop computational programmes for DNA analysis, and established the foundation of DDBJ, the DNA databank of Japan.

He made every effort to found the Biophysical Society of Japan and led the International Conference of Biophysics, held in Kyoto in 1978, to success as the chairman of the executive committee. From 1980 to 1981, he served as the president of the Biophysical Society of Japan to do his best in developing the biophysical field in Japan and internationalizing the Society. He also contributed largely to the development of the research field by holding international symposia many times. For his great academic and educational contributions, Dr. Ooi was awarded the Third Class of the Order of the Rising Sun in November, 2002.



PUBLICATIONS
THESES

PUBLICATIONS

STATES AND STRUCTURES

I. Atomic and Molecular Physics

Mihara H, Fujii T, Kato S, Kurihara T, Hata Y, Esaki N: Structure of External Aldimine of *Escherichia coli* CsdB, an IscS/NifS Homolog: Implications for Its Specificity toward Selenocysteine, *J. Biochem.*, **131**, 679-685 (2002).

Hata Y, Fujii T, Hayashida Y, Aso Y, Ishiguro M: Crystal Structures of Three Lectins from the Roots of Pokeweed, *Acta Cryst.*, **A58**(Supplement), C292 (2002).

Fujii T, Sakai H, Kawata Y, Hata Y: Crystal Structure of Thermostable Aspartase and Exploration of Functional Sites in Aspartase Family, *Acta Cryst.*, **A58**(Supplement), C100 (2002).

Fujii T, Hata Y: Crystal Structure Analysis of Thermostable Aspartase and Exploration of Functional Sites, *The Journal of Structural Biology Sakabe Project*, 8(2)1-9 (2002) (in Japanese).

Olariu S, Olariu A, Ito Y, Mukoyama T: Cross-sections for the Electron Excitation of γ -ray Fluorescence, *Nucl. Instrum. & Methods B*, **179**, 11-14 (2001).

Tochio T, Ito Y, Omote K: Broadening of the X-ray Emission Line Due to the Instrumental Function of the Double-crystal Spectrometer, *Phys. Rev. A*, **65**, 04502-1~6 (2002).

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Ito Y, Tochio T, OoHashi H, Shigeoka N, Vlaicu M A, Kaneyoshi T, Motoyama M, Shoji T, Fukushima S: A Trial Fitting on $K\alpha_{1,2}$ Emission Spectra in Transition Metal, *Proceedings of International Seminar on Photoionization in Atom, Kyoto University Press*, 66-73 (2002).

Shigeoka N, OoHashi H, Ito Y, Tochio T, Vlaicu M A, Nisawa A, Yoshikawa H, Fukushima S, Watanabe M: The Behavior of Fe $K\alpha$ satellites around the threshold, *Proceedings of International Seminar on Photoionization in Atom, Kyoto University Press*, 80-84 (2002).

OoHashi H, Shigeoka N, Tochio T, Ito Y, Vlaicu M A, Nisawa A, Yoshikawa H, Fukushima S, Watanabe M: Contribution of Indirect Ionization of Au $L\beta_2$ Satellites, *Proceedings of International Seminar on Photoionization in Atom, Kyoto University Press*, 85-88 (2002).

Vlaicu M. A, Ito Y, Shigeoka N, OoHashi H, Fukushima S, Yoshikawa H, Nisawa A: Photo-excitation of Multi-electron Transitions in Heavy Elements by Synchrotron Radiation, *Proceedings of International Seminar on Photoionization in Atom, Kyoto University Press*, 62-65 (2002).

Ito Y, Shigeoka N, OoHashi H, Tochio T, Vlaicu M. A, Nisawa A, Yoshikawa H, Fukushima S: X-ray Emission Spectroscopy around the Threshold in 3d and Heavy Elements, *Ion Transport in Ionic Conductors Proceedings of the 6th Forum on Superionic Conductor Physics*, 1-6 (2002).

Fukushima S, Ito Y: The Investigation on the Relaxation of Inner-shell Induced by Tunable X-ray of the Third Generation SR, *Materia Japan*, **41**, 707-712 (2002) (in Japanese).

Yoshikado S, Ito Y, Reau J M: Fluoride on Conduction in $Pb_{1-x}Sn_xF_2$ Solid Solution System, *Solid State Ionics* **154/155** (2002) 503-509.

Uda M, Yamashita D, Terashi D, Yamamoto T, Osawa H, Kanai K, Nakamatsu H, Perera R: XANES Spectra of Sesqui-oxides of Al, Cr and Fe, *J. Electron Spectrosc. Relat. Phenom.*, **114-116**, 819-823 (2001).

Tsuji J, Kojima K, Ikeda S, Nakamatsu H, Mukoyama T, Taniguchi K: Li K-edge Spectra of Lithium Halides, *J. Synchrotron Radiat.*, **8**, 554-556 (2001).

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II. Electron Microscopy and Crystal Chemistry

Suga T, Isoda S, Moriguchi S, Kobayashi T: Vacuum-deposited Thin Films of $(\mu\text{-Oxo})\text{bis}[(\text{phthalocyaninato})\text{aluminum(III)}]$ ($(\text{AlPc})_2\text{O}$), *Mol. Cryst. Liq. Cryst.*, **370**, 253-256 (2001).

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Maeda T, Isoda S, Kobayashi T: Epitaxial Growth and Defect Structure of Quaterylene Studied by High Resolution Electron Microscopy, *Physica Status Solidi*, **191**, 489-498 (2002).

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Takajo D, Fujiwara E, Irie S, Nemoto T, Isoda S, Ozaki H, Toda N, Tomii S, Magara T, Mazaki Y, Yamamoto G: Monolayer and Bilayer Formation of 17,19-Dotetracontadiyne at a Liquid/solid Interface, *J. Cryst. Growth*, **237-239**, 2071-2075 (2002).

Yaji T, Izumi K, Isoda S: Comparative Study on Surface Morphology by Photo- and Thermal-polymerization of a Diacetylene, *Appl. Surf. Sci.*, **188**, 519-523 (2002).

Nagasawa H, Maruyama M, Komatsu T, Isoda S, Kobayashi T: Physical Characteristics of Stable Silver Nanoparticles Formed Using a New Thermal-Decomposition Method, *phys. stat. sol., (a)* **191**, 67-76 (2002).

Nemoto T, Takajo D, Isoda S: Structures of the Initial Adsorbed Layers of Stearic Acid at Liquid/solid Interface, *Acta Cryst. (Suppl)*, **A58**, C361 (2002).

Isoda S, Kuwamoto K, Ogawa T: Experimental Estimation of Dynamical Scattering Effect on Electron Crystallography, *Acta Cryst. (Suppl)*, **A58**, C173 (2002).

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Futaesaku Y, Isoda S: Elemental Mapping, *Denshi-kennbikyoku*, **37**, 7 (2002) (in Japanese).

Isoda S, Kobayashi T: Epitaxial Growth of Huge Molecules, *Frontier of Epitaxial Growth (Kyoritu-Syuppan)*, **4**, 161-177 (2002) (in Japanese).

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Sasase M, Okayasu S, Kurata H, Hojou K: Defect Structure of High-Tc Superconductor by High-energy Heavy Ion Irradiation, *J. Electron Microsc.*, **51**, S235-S238 (2002).

Morikawa H, Matsusaka K, Kurata H, Yoshino Y: The Build-up Process of (111) Pole of a Tungsten Tip and the Shape Change of a Tip Cap, *J. Vac. Soc. Jpn.*, **44**, 36-41 (2001) (in Japanese).

Kurata H: EELS Imaging, *Denshi-kennbikyoku*, **36**, 217-219 (2001) (in Japanese).

Kurata H: Elemental Mapping: Introduction, *Denshi-kennbikyoku*, **37**, 8-9 (2002) (in Japanese).

III. Polymer Condensed States

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MOLECULAR BIOLOGY AND INFORMATION

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“Studies on the Sol-Gel Synthesis of Ceramics and Dye-doped Glasses Aiming at Advanced Optical Devices”
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D Sc, Kyoto University
“Circulation of Trace Elements in Lake Biwa”
Supervisor: Prof SOHRIN, Yoshiki
25 March 2002

Mohamed ALMOKHTAR M. Abdel-Mola
D Sc, Kyoto University
“Magnetism of Cr Thin Films with ^{119}Sn Monolayers in Fe/Cr and V/Cr Multilayers”
Supervisor: Assoc Prof MIBU, Ko
23 January 2002

MOMOSE, Yashima
D Pharm Sc, Kyoto University
“Studies on Kinetic Resolution by Nucleophilic Catalysis with Chiral Pyrrolidinopyridines”
Supervisor: Prof FUJI, Kaoru
25 March 2002

MORITA, Akio
D Sc, Kyoto University
“Evaluation of Combined-Function Synchrotron based on High-Precision Magnetic Field Measurements”
Supervisor: Prof NODA, Akira
25 March 2002

NIIDA, Haruki
D Eng, Kyoto University
“Studies on Organic-Inorganic Hybrid Low-Melting Oxide-Based Glasses”
Supervisor: Prof YOKO, Toshinobu
25 March 2002

NURUZZAMAN, Mohammnd
D Pharm Sc, Kyoto University
“Use of 1,1'-Binaphtyl Derivatives in Asymmetric Synthesis and Enantiomeric Recognition”
Supervisor: Prof FUJI, Kaoru
25 March 2002

OHASHI, Yohei
D Sc, Kyoto University
“Functional Analysis of an *Arabidopsis* Homeobox Gene, *GLABRA2*”
Supervisor: Prof OKA, Atsuhiko
25 March 2002

OHNISHI, Hiroshi
D Pharm Sc, Kyoto University
“Studies on Asymmetric Reactions with 8,8'-Disubstituted-1,1'-Binaphtyls”
Supervisor: Prof FUJI, Kaoru
25 March 2002

SAITO, Takashi
D Sc, Kyoto University
“Single Crystal Growth and the Physical Properties of a One Dimensional Spin Gap Compound, High Pressure Phase of $(\text{VO})_2\text{P}_2\text{O}_7$ ”
Supervisor: Prof TAKANO, Mikio
25 May 2002

SUGIMURA, Takashi
D Sc, Kyoto University
“Pulse Stretcher of Election Beam with use of Third Order Resonance and RF Knockout Method”
Supervisor: Prof NODA, Akira
25 March 2002

TAKENAKA, Keisi
D Sc, Kyoto University
“Synthesis of Optically Active Propargyl Alcohol Derivatives Using Lipase”
Supervisor: Assoc Prof NAKAMURA, Kaoru
23 July 2002

TOCHIO, Tatsunori
D Sc, Kyoto University
“Broadening of the X-ray Emission Line due to the Instrumental Function of the Double-crystal Spectrometer”
Supervisor: Assoc Prof ITO, Yoshiaki
24 March 2002

YAMAGUCHI, Hitomi
D Sc, Kyoto University
“Asymmetric Reduction of Keto Esters with Actinomycetes”
Supervisor: Assoc Prof NAKAMURA, Kaoru
25 March 2002

YAMAMOTO, Hiroyuki
D Eng, Kyoto University
“Studies on Structure of Native Cellulose by High-Resolution Solid-State ^{13}C NMR Spectroscopy”
Supervisor: Prof HORII, Fumitaka
25 March 2002



**SYMPOSIUM OF
GRADUATE STUDENTS**

SEMINARS

**MEETINGS AND
SYMPOSIUMS**



SYMPOSIUM OF GRADUATE STUDENTS

(21 February 2003)

Doctoral Course Students (Oral Presentations)

SHIGEOKA, Nobuyuki (STATES AND STRUCTURES I)
"Investigation of X-ray satellites on Fe and Ti"

MIYAKE, Kousaku (SOLID STATE CHEMISTRY I)
"Magnetic structure and magnetoresistance effect of a magnetic domain wall in nano-contact structures"

ISHIWATA, Shintaro (SOLID STATE CHEMISTRY III)
"Synthesis and Crystal Growth under High Pressure for Transition Metal Oxides with Perovskite-type Structure and Charge Disproportionation"

AKITA, Yosuke (SOLID STATE CHEMISTRY IV)
"Optical dielectric multilayer structures with a dual-periodicity"

MORI, Ryohei (SOLID STATE CHEMISTRY IV)
"Preparation and photoelectrochemical/photocatalytic properties of sol-gel derived TiO₂ thin film with spinodal phase separation structure."

MIYAZAKI, Tsukasa (FUNDAMENTAL MATERIAL PROPERTIES II)
"X-ray and neutron reflectivity study of polyimide thin films swollen by hydrocarbon gases"

WAKAMIYA, Atsushi (ORGANIC MATERIALS CHEMISTRY II)
"Structure and Properties of Cationic Species of Sulfur-Containing Cyclic π -Conjugated Systems Surrounded by Rigid σ -Frameworks"

SHIRASAKA, Toshiaki (SYNTHETIC ORGANIC CHEMISTRY I)
"Photophysical Properties Control of π -Electron Systems Containing Main-Group Elements"

SAEKI, Tomoyuki (SYNTHETIC ORGANIC CHEMISTRY I)
"Reactivity of Silylenes Intramolecularly Coordinated by Group 15 and 16 Elements"

OTSUBO, Tadamune (SYNTHETIC ORGANIC CHEMISTRY II)
"Synthesis and Functions of Homooxalix[3]arene Derivatives"

NAGATA, Kazuto (BIOORGANIC CHEMISTRY I)
"Studies on the Synthesis and Properties of the Disulfur and Diselenium Complexes of Platinum Utilizing New Bulky Phosphine Ligands"

NAKATA, Norio (BIOORGANIC CHEMISTRY I)
"Synthesis and Properties of Kinetically Stabilized Germaaromatic Compounds"

YAMANAKA, Rio (BIOORGANIC CHEMISTRY I)
"Asymmetric reduction of ketones by photosynthetic organisms"

NOMURA, Akiko (BIOORGANIC CHEMISTRY II)
"Redesign of the Metal Coordination Sites in the Zinc Finger Peptides"

SUZUKI, Tomoki (BIOORGANIC CHEMISTRY II)
"Arginine-rich peptides: novel candidates for carrier molecules

and their mysterious internalization mechanism"

BAHK, Songchul (BIOORGANIC CHEMISTRY III)
"*In situ* detection of metals in Alzheimer's disease brains by scanning electron microscope with energy dispersive X-ray spectrometry"

FUJII, Ryota (MOLECULAR BIOFUNCTION I)
"Directed evolution of lipase for altering reaction specificity"

Master's Course Students (Poster Presentations)

MINARI, Takeo (STATES AND STRUCTURES II)
"Device structures and interface transport properties of an organic thin film transistor"

MIYAMOTO, Yusuke (STATES AND STRUCTURES II)
"Kinetic and morphological studies on desorption of organic molecules"

YOSHIOKA, Yasutomo (STATES AND STRUCTURES II)
"TEM observation of Grätzel dye adsorbed TiO₂"

NAKAYA, Yuichi (STATES AND STRUCTURES III)
"Ion-conducting Behavior of the Composites from Branched Poly(oxyethylene) and Oxysulfide Glass"

TANI, Kenji (STATES AND STRUCTURES III)
"Novel composite type solid electrolyte from lithium triborate glass and poly(oxyethylene)"

USUI, Yuma (INTERFACE SCIENCE I)
"NMR study of dehalogenation and decarboxylation reactions of aromatic compounds in supercritical water"

TSUNASHIMA, Hiroyuki (INTERFACE SCIENCE I)
"NMR Study of Electrolyte Aqueous Solutions at High Temperatures"

HIRAMATSU, Takaaki (INTERFACE SCIENCE II)
"Syntheses and characterization of new amphoteric and polar molecules fabricated by connecting donor and acceptor segments with a quinoid bridge"

TSUTSUMI, Jun'ya (INTERFACE SCIENCE II)
"Correlation of aggregation structure and electronic properties of zwitterionic molecules"

YOSHIDA, Tadashi (INTERFACE SCIENCE II)
"Comparison of electronic structures in triphenodithiazine thin films vacuum-deposited at different substrate temperatures"

KURAHASHI, Kensuke (INTERFACE SCIENCE III)
"Solvent extraction study of divalent transition metal ions with chelating ligand bearing crownether moiety"

MATSUMOTO, Hirofumi (INTERFACE SCIENCE III)
"Synergistic extraction of metal ions with polydentate neutral ligand having phosphine oxide moiety"

MIKATA, Michi (INTERFACE SCIENCE III)

“The development of the analytical method for dissolved Zr, Nb, Hf, Ta, and W in seawater and their vertical profiles in the Western North Pacific Ocean”

IJKO, Norihiro (SOLID STATE CHEMISTRY I)

“Growth-Orientation Dependence of Cr magnetism in Fe/Cr and Cr/Sn Multilayers”

MIZUTANI, Masahiro (SOLID STATE CHEMISTRY I)

“Perpendicular giant magnetoresistance in line-shaped magnetic trilayers”

OHKOCHI, Takuo (SOLID STATE CHEMISTRY I)

“Research on the magnetism of Gd/Cu multilayers using X-ray and γ -ray resonance”

CHUREI, Taichiro (SOLID STATE CHEMISTRY II)

“Effect of Magnetic-impurities on Superconductivity and Spin fluctuation of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ”

IKEUCHI, Kazuhiko (SOLID STATE CHEMISTRY II)

“New Approach for Carrier Doping Effect about $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ”

KUROSHIMA, Shinichi (SOLID STATE CHEMISTRY II)

“Phase diagram of electron-doped high- T_c superconductor”

KAN, Daisuke (SOLID STATE CHEMISTRY III)

“Preparation and optical properties of CaCuO_2 thin film with the infinite layer structure”

KOBINO, Masashi (SOLID STATE CHEMISTRY III)

“Structure and Properties of the [Ca-Fe] hydrotalcite”

YAMADA, Ikuya (SOLID STATE CHEMISTRY III)

“High pressure synthesis and physical properties of transition metal perovskites and related compounds — singlecrystal growth of BiMnO_3 and magnetic phase diagram of $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ —”

SAKOH, Akifumi (SOLID STATE CHEMISTRY IV)

“Photochemical process of divalent germanium in GeO_2 - SiO_2 glasses responsible for photorefractive index change”

MIYABE, Daisuke (SOLID STATE CHEMISTRY IV)

“Local structure of six-fold coordinated silicon and aluminum in alkali phosphate glasses”

MIZUNO, Megumi (SOLID STATE CHEMISTRY IV)

“Studies on the structure of lead silicate glasses — From the viewpoint of leaching behavior of Pb^{2+} —”

KADOYA, Hidenori (FUNDAMENTAL MATERIAL PROPERTIES I)

“Electric Birefringence and Viscoelasticity of Amorphous Polymers”

OH, Gwan-Kyo (FUNDAMENTAL MATERIAL PROPERTIES I)

“Dynamic Birefringence and Viscoelasticity of Polycarbonates”

OISHI, Yohei (FUNDAMENTAL MATERIAL PROPERTIES I)

“Viscoelasticity of Biantionic Polymer”

FUKUSHIMA, Hajime (FUNDAMENTAL MATERIAL PROPERTIES II)

“Polymer Crystallization Process under Shear by Depolarized Light Scattering Method”

OGINO, Yoshiko (FUNDAMENTAL MATERIAL PROPERTIES II)

“Crystallization of Isotactic Polypropylene under Shear Flow”

OKUYAMA, Tomohiro (FUNDAMENTAL MATERIAL PROPERTIES II)

“Freezing of Structure in the Induction Period for the Melt-crystallization of Poly(ethylene terephthalate)”

INUI, Nobuhiko (FUNDAMENTAL MATERIAL PROPERTIES III)

“Analysis of Local Structure in an Amorphous Polyester by Two-Dimensional Double-Quantum NMR”

NISHIMURA, Takuya (FUNDAMENTAL MATERIAL PROPERTIES III)

“Influences of copolymer composition or tacticity on the structure and dynamics of polymer materials”

ONODERA, Gen (FUNDAMENTAL MATERIAL PROPERTIES III)

“Dynamics of Cellulose Acetates in Dilute Solution”

KWAK, Yungwan (ORGANIC MATERIALS CHEMISTRY I)

“Kinetic studies on the activation mechanisms in organotelluride-mediated living radical polymerization”

MARUTANI, Eizo (ORGANIC MATERIALS CHEMISTRY I)

“Controlled Graft Polymerization on the Surface of Magnetic Particle by Living Radical Polymerization Technique”

IDOMOTO, Yuichi (ORGANIC MATERIALS CHEMISTRY II)

“Synthesis of a Tripod-Shaped Trithiol Containing an Adamantane Framework and Preparation of Its Monolayer on Au Surface”

MIYATA, Yasuo (ORGANIC MATERIALS CHEMISTRY II)

“Synthesis and Properties of π -Conjugated Oligomers Composed of Alternately Connected Furan and Thiophene”

MURATA, Michihisa (ORGANIC MATERIALS CHEMISTRY II)

“Synthesis of Open-Cage and Endohedral Fullerene Derivatives”

FUJIMURA, Hirokazu (SYNTHETIC ORGANIC CHEMISTRY I)

“Synthesis and Reactions of 1,6-Digerm- and 1-Germa-6-sila[4.4.4]propellane and Their Derivatives”

KATAOKA, Takeshi (SYNTHETIC ORGANIC CHEMISTRY I)

“New Si-Te Bond Cleavage Routes to Silyllithium Compounds: The First Example of Tellurium-Substituted Silyllithium”

HIRASE, Keizo (SYNTHETIC ORGANIC CHEMISTRY II)

“Structure and Properties of RS-lactic oligomers”

MORIKAWA, Hiroshi (SYNTHETIC ORGANIC CHEMISTRY II)

“Efficient synthesis of optically active polynaphthalenes”

NAGAOKA, Yoshie (SYNTHETIC ORGANIC CHEMISTRY II)

“Selective Reactions promoted by a new class of chiral nucleophilic catalysts”

MIZUHATA, Yoshiyuki (BIOORGANIC CHEMISTRY I)

“Synthetic Studies of Novel Silacumulenes by Taking Advantage of Steric Protection”

HADA, Shintaro (BIOORGANIC CHEMISTRY II)

“Design of DNA-binding single zinc finger protein”

KONDO, Yumi (BIOORGANIC CHEMISTRY II)
“Influence of amino acid numbers between two ligand cysteines of zinc finger proteins on affinity and specificity of DNA binding”

SHIRAIISHI, Yasuhisa (BIOORGANIC CHEMISTRY I)
“Design of Novel Zinc Finger Protein Recognizing Complementary Strand”

KAI, Kosuke (MOLECULAR BIOFUNCTION I)
“Induction of coumarins in morning glory after treatment with non-pathogenic *Fusarium*”

NOGUCHI, Etsuko (MOLECULAR BIOFUNCTION I)
“Immunochemical characterization of tea leaf β -primeverosidase, a key enzyme in tea aroma formation”

OHNISHI, Toshiyuki (MOLECULAR BIOFUNCTION I)
“Functional analysis of cytochrome P450 monooxygenase involved in brassinosteroid catabolism”

OKUTSU, Reiko (MOLECULAR BIOFUNCTION I)
“A rapid and facile determination of aglycon specificity of glycosidases by using competing substrates”

TACHI, Norihito (MOLECULAR BIOFUNCTION I)
“Synthetic study on transition-state analogue inhibitors of γ -glutamyltranspeptidase”

YAMAGUCHI, Ayako (MOLECULAR BIOFUNCTION I)
“Functional characterization of cytochrome P450 *CYP78A* involved in plant hormone homeostasis”

AKABORI, Manami (MOLECULAR BIOFUNCTION II)
“Structure and Function of a Novel Amino Acid Dehydrogenase Catalyzing Reductive Amination of Glyoxylate”

KAKUTANI, Ryo (MOLECULAR BIOFUNCTION II)
“*N*-Methyl amino acid dehydrogenase from *Pseudomonas putida* : A novel biocatalyst applicable to the synthesis of optically active *N*-substituted amino acids”

KOZAKI, Maiko (MOLECULAR BIOFUNCTION II)
“Studies of chlorophenylserine decarboxylase”

KUWANA, Eriko (MOLECULAR BIOFUNCTION II)
“Studies of distribution and dynamism of essential trace element selenium in mouse brain”

MARUOKA, Naruyuki (MOLECULAR BIOFUNCTION II)
“Studies of Iron-Sulfur Cluster Biosynthesis in *Synechocystis* sp. PCC6803”

OGAWA, Shin-ichiro (MOLECULAR BIOFUNCTION II)
“Role of cysteine residues of mouse selenocysteine lyase”

IMAI, Kumiko (MOLECULAR BIOLOGY AND INFORMATION II)
“Analysys of the expression and function of AtCDKA;1 expressed in Trichome of Arabidopsis”

IWAKOSHI, Shintaro (MOLECULAR BIOLOGY AND INFORMATION II)
“Possibility of integration of cytokinin signal and ethylene signal in *arabidopsis* His-Asp phosphorelay signal transduction system”

FUJITA, Masashi (BIOINFORMATICS CENTER I)
“Weak similarity detection method for protein tertiary structure prediction”

MORIYA, Yuhki (BIOINFORMATICS CENTER I)
“Evaluation of Sequence Alignment Score by Statistics”

OKUDA, Shujiro (BIOINFORMATICS CENTER I)
“Prediction of operons based on microarray data in *Bacillus subtilis*”

YAMADA, Rikuhiro (BIOINFORMATICS CENTER I)
“Application of G.A to Bifurcation Analysis and Analysis of Circadian Rhythm”

YAMADA, Takuji (BIOINFORMATICS CENTER I)
“Extraction of modules from metabolic pathway with phylogenetic profile”

FUKAGAWA, Daiji (BIOINFORMATICS CENTER II)
“A Performance Analysis of a Greedy Algorithm for Inferring Boolean Networks”

K.C., Dukka Bahadur (BIOINFORMATICS CENTER II)
“Protein Side Chain Packing Using an Efficient Maximum Clique Algorithm”

SAIGO, Hiroto (BIOINFORMATICS CENTER II)
“Protein Homology Detection Using Sequence Alignment and Support Vector Machines”

SHIBATA, Yuzo (BIOINFORMATICS CENTER II)
“Valuation system for unused gene patents by using time series data of literature and real options”

YAMAMURA, Masaki (BIOINFORMATICS CENTER II)
“Sequence Analysis of PDZ Domains toward Their Binding Partner Prediction”

FUJIMOTO, Shinji (NUCLEAR SCIENCE RESEARCH FACILITY I)
“Non-destructive electron beam profile measurement with Micro Channel Plate(MCP)”

YAMAZAKI, Atsushi (NUCLEAR SCIENCE RESEARCH FACILITY I)
“X-ray production with backward-Compton scattering at KSR”

SEMINARS

Prof AOI, Keigo
Graduate School of Bioagricultural Sciences, Nagoya, Japan
“Synthesis and Functionality of Dendrimers”
23 April 2002

Dr AOKI, Hiroyuki
Graduate School of Engineering, Kyoto University, Kyoto, Japan
“Two-Dimensional Phase-Separation of Polymer Monolayer Studied by Scanning Near-Field Optical Microscopy”
13 January 2002

Prof BAEUERLE, Peter
Department of Organic Chemistry II, University of Ulm, Ulm, Germany
“Functional pi-Electron Materials”
19 November 2002

Prof BELOKON, Yuri N.
Russian Academy of Science, Russia
“Novel Chiral Phase Transfer Catalysts for Asymmetric C-C Bond Formation Reactions”
8 January 2002

Lect BISHOP, Gerard
Institute of Biological Sciences, University of Wales Aberystwyth, UK
“The Biosynthesis and Signal Transduction of Plant Steroid Hormones”
29 January 2002

Prof BUBACK, Michael
Georg-August-Universitaet Goettingen, Germany
“Initiation and Termination Processes in Free-Radical Polymerization”
15 July 2002

Prof Dr BUCKEL, Wolfgang
University of Marburg, Germany
“Radicals in Enzymatic Catalysis: Coenzyme B12 as a Radical Generator and ATP-Induced Electron Transfer”
2 July 2002

Prof CEULEMANS, Arnout
Division of Quantum Chemistry, University of Leuven, Belgium
“Quantum Chemistry of Carbon Cages and Networks: The Tetrahedral Family of (3,6) Cages”
11 January 2002

Prof DE LESQUEN, Alain
Nuclear Research Institute, Saclay, CNRS, France
“Recent Results of the Underground Dark Matter Search EDELWEISS”
7 August 2002

Assoc Prof DI NOTO, Vito
University of Padova, Padova, Italy
“Zeolitic Inorganic-Organic Polymer Electrolytes : Synthesis, Characterization and Ionic Conductivity of a Material Based on Oligo (Ethylene Glycol) 600, (CH₃)₂ SnCl₂ and K₄Fe(CN)₆”
8 February 2002

Prof DOI, Yoshiharu
Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology, Yokohama, Japan
“Developments of Biodegradable Polymers (Green Polymers): Their Problems and Prospects”
7 March 2002

Prof DOUGLAS, Kenneth T.
The University of Manchester, Manchester, UK
“Inhibitors of Thymidine Phosphorylase”
7 November 2002

Prof DURNY, Rudolf
Slovak Technical University, Bratislava, Slovakia
“Correlation between the Results of Charge DLTS and ESR Techniques Obtained on Undoped Hydrogenated Amorphous Silicon”
13 March 2002

Prof ENDERS, Dieter
Institute für Organische Chemie der RWTH Aachen, Aachen, Germany
“New Methods for Asymmetric Synthesis of Bioactive Compounds”
10 October 2002

Prof GOEDRL, Werner A.
Universitaet Ulm, Germany
“Structure and Thermodynamics of Monolayers of a Melt Polymer Brush”
26 March 2002

Prof GUENET, Jean-Michel
Institute Charles Sadron, CNES, France
“Thermoreversible Gels as Encapsulating Media for Magnetic Materials”
26 April 2002

Prof HAMA, Hiroyuki
LNS, Tohoku University, Japan
“Present Status and Future Plan of Electron Linac at LNL, Tohoku University”
29 March 2002

Dr HE, Hanhong
Donghua University, China
“Formation of PET Composite Fibers Containing Thermotropic Liquid Crystalline Polymers”
28 October 2002

Dr HORIKOSHI, Satoshi
Frontier Research Center for the Global Environment Protection, Meisei University, Japan
“Degradation of Organic Pollutants by an Integrated Photocatalyzed Oxidation Method”
6 June 2002

Prof HOSONO, Kazuhiko
LASTI, Himeji Institute of Technology, Japan
“High Energy Gamma-Ray Source by Laser Inverse Compton scattering and the application at NewSUBARU”
29 March 2002

Dr IGNATOVICH, Lubov
Latvian Institute of Organic Synthesis, Latvia
“Aryl- and Hetarylgermatranes”
11 October 2002

Prof JAESCHKE, Eberhard
BESSY, Germany
“BESSYII and Future Plans - FEL and a Dedicated Small Ring”
30 April 2002

Prof KAKINUMA, Katsumi
Department of Chemistry, Tokyo Institute of Technology, Japan
“Molecular Analysis and its Application of Secondary Metabolism in Microorganism”
5 March 2002

Dr KATO, Hiroaki
Kinetic Crystallography Research Team, Membrane Dynamics Research Group, Harima Institute at SPring-8, RIKEN, Japan
“Ultra-High Resolution Analysis of X-ray Crystal Structure of Endopolygalacturonase and its Enzymatic Mechanism”
11 March 2002

Prof KAWAGUCHI, Haruma
Keio University, Tokyo, Japan
“Synthesis and Function of Environment-Responsive Particles”
25 March 2002

Prof KIKUTANI, Takeshi
Tokyo Institute of Technology, Tokyo, Japan
“Orientation Induced Crystallization in Polymer Processing”
29 March 2002

Dr KIM, Eun-San
PAL, Pohang University of Science and Technology, Korea
“Beam Dynamics in PLS Storage Ring”
6 March 2002

Dr KIM, Eun-San
PAL, Pohang University of Science and Technology, Korea
“Report on Accelerator Physics Studies in PLS”
29 October 2002

Prof KUBO, Kenya
College of Liberal Arts, International Christian University, Japan
“Muon and Muonium Chemistry”
28 November 2002

Prof LEMKE, Frederick R.
Department of Chemistry and Biochemistry, Ohio University, USA
“Interaction of Silanes with Ruthenium Complexes: Spectroscopic, Structural and Catalysis Studies”
8 July 2002

Prof LUKEVICS, Edmunds
Latvian Institute of Organic Synthesis, Latvia
“Three Neighbours: Carbon, Silicon, Germanium. Chemical and Biological Similarities and Differences.”
11 October 2002

Prof MATHON, George
City University, London, UK
“Current-Driven Switching of the Magnetization in Magnetic Multilayers”
30 September 2002

Prof MATSUOKA, Shiro
Polytechnic University, Brooklyn, NY, USA
“Glassy State from Irreversible Thermodynamic Viewpoints”
4 July 2002

Prof MICHL, Josef
University of Colorado at Boulder, USA
“A ‘Tinkertoy’ Molecular Construction Kit for Molecular Electronics”
18 October 2002

Dr MIDDENDORF, H. D.
Clarendon Laboratory, University of Oxford, UK
“Evolution of the Energy Landscape of Protein from 20 to 270K”
17 January 2002

Dr MINAKAWA, Masayuki
National Research Institute of Fisheries Science, Yokohama, Japan
“Dynamics of Mn and Al in the Marginal Seas”
14 February 2002

Assoc Prof MITANI, Seiji
Institute for Materials Research, Tohoku University, Japan
“Tunneling Magnetoresistance in Granular Thin Films - From Basics to Applications - I”
5 November 2002

Assoc Prof MITANI, Seiji
Institute for Materials Research, Tohoku University, Japan
“Tunneling Magnetoresistance in Granular Thin Films - From Basics to Applications - II”
10 December 2002

Dr MÖHL, Dieter
CERN, Switzerland
“Accumulation of Antiprotons with Stochastic Cooling”
26 April 2002

Prof MUELLEN, Klaus
Max-Planck Institute for Polymer Materials, Mainz, Germany
“Molecular Graphite”
27 September 2002

Dr NAKA, Takehiko
Takeda Analytical Research Laboratories, Ltd, Osaka, Japan
“Research and Development of a Novel Antihypertensive Agent: Nonpeptide Angiotensin II Receptor Antagonist, Candesartan Cilexetil”
11 June 2002

Prof NEGISHI, Eiichi
Purdue University, USA
“Zr-Catalyzed Enantioselective Carboalumination of Unactivated Alkenes”
16 October 2002

Prof OGAWA, Kazufumi
Department of Advanced Materials Science, Faculty of Engineering, Kagawa University, Takamatsu, Japan
“Preparation of Monomolecular Films and the Control of Orientation and Arrangement of Molecules in those Films”
19 July 2002

Prof OGAWA, Kazufumi
Department of Advanced Materials Science, Faculty of Engineering, Kagawa University, Takamatsu, Japan
“Applications of Monomolecular Films: Inclusion of Various Functions”
11 October 2002

Mr OKABE, Kota
Hiroshima University, Japan
“Resonance Instability of High Intensity Ion Beam”
25 February 2002

Dr OKAMURA, Haruyuki
Department of Applied Chemistry, Osaka Prefecture University,
Osaka, Japan
“Synthesis of Random and Block Copolymers of Styrene and
Styrenesulfonic Acid with Low Polydispersity Using Nitroxide-
Mediated Living Radical Polymerization Technique”
13 January 2002

Prof P.A. Berg Georg
Kernfysisch Versneller Instituut, University of Groningen,
Netherlands
“Magnetic Analysis and Matching Techniques in Nuclear
Physics”
3 December 2002

Prof PACKER, Jeffrey
University of Toronto, Canada
“Polymer Materials in Civil Engineering”
8 June 2002

Prof RANGAPPA, K. S.
University of Mysore, India
“Crystal and Molecular Structure Studies of Nitrenium Ions”
10 October 2002

Prof RAO, Chintamani Nagesa Ramachandara
Jawaharlal Nehru Centre for Advanced Scientific Research, India
“Basic Building Units and the Building Up Process in Open-
Framework Architectures”
11 March 2002

Prof RISEN Jr, William M
Brown University, Providence, USA
“Novel Polyurethane Ionomers and a Study of Their Physical
and Chemical Properties”
18 November 2002

Prof RUBIN, Yves
Department of Chemistry and Biochemistry, University of
California, Los Angeles, USA
“Chemistry of C₆₀ and Approaches to Endohedral Metallo-
fullerenes”
6 April 2002

Prof SAKABE, Shuji
ILE, Osaka University, Japan
“Interaction between Matter and Ultra High Intensity and Short
Pulse Laser”
30 September 2002

Dr SAKAMOTO, Shinichi
Center for Proton Accelerator Facilities, Tokai Research
Establishment, Japan Atomic Energy Research Institute, Japan
“Development of New Elemental Analysis Method “dreamX”
with Muonic X-rays for Historical Relics”
28 November 2002

Dr SCHELER, Ulrich
Institut fuer Polymerforschung, Doersden e. V., Germany
“Solid-State and Electrophoresis NMR of Functionalized
Polymers”
27 November 2002

Dr SCHLETTWEIN, Derck
Department of Chemistry, Physical Chemistry 1, University of
Oldenburg, Oldenburg, Germany
“Design of Molecular Interactions to Control the Architecture
of Thin Organic Films”
13 August 2002

Dr SEGAL, David J.
The Scripps Research Institute, La Jolla CA, USA
“Novel Zinc Finger Proteins for the Therapeutic Regulation and
Modification of Genes”
18 June 2002

Prof SHOJI, Akira
Faculty of Engineering, Gunma University, Kiryu, Japan
“Synthesis and Solid-State NMR Studies of Model Polypeptides”
5 February 2002

Dr SINGH, M
QSS Group, Inc., NASA Glen Research Center, Cleveland, USA
“Opportunities and Challenges in the Applications of Advanced
Ceramics and Composites in the New Millennium”
24 May 2002

Prof STEUDEL, Ralf
Institute for Inorganic and Analytical Chemistry, Technical
University of Berlin, Germany
“Modern Synthesis of Organic Polysulfanes and Structures of
Sulfur-Rich Chains and Rings”
10 April 2002

Assoc Prof SUGIHARA, Takuminchi
Faculty of Pharmaceutical Sciences, Tokushima Bunri University,
Tokushima, Japan
“Relationship of Reactivity, Structure, and Ligand Effect in
Cobalt Carbonyl Complexes”
11 June 2002

Prof SUGITA, Satoshi
Guanajuato University, Mexico
“Reactivity of Alumina”
5 December 2002

Dr SYRESIN, Evgeny
JINR, Dubna, Russia
“Peculiarity of Electron Cooling at Low Ion Energy in Small
Storage Ring”
7 February 2002

Dr SYRESIN, Evgeny
JINR, Dubna, Russia
“Electron Cooling and Related Problems in LSR Project”
26 August 2002

Dr TABATA, Satoshi
Kazusa DNA Research Institute, Japan
“Genome Analysis of *Lotus japonicus*”
23 May 2002

Dr TAKADA, Akihiko
Interdisciplinary Graduate School of Engineering Sciences,
Kyushu University, Fukuoka, Japan
“Viscoelasticity of Potassium Neutralized Telechelic
Poly(ethylene butylene) Ionomer Solutions in Non-polar
Solvent”
13 January 2002

Dr TAKEDA, Kenji
ERATO, Japan
“The State of the Arts and Future Prospects of Polymer Small
Sphere Laser”
8 March 2002

Prof TANABE, Tetsumi
KEK, Japan
“Electron Cooling and Atomic Collision Experiment at Storage
Ring TARN II”

14-15 February 2002

Prof TERAOKA, Hirobumi
Medical Research Institute, Tokyo Medical and Dental
University, Tokyo, Japan
“Hepatocyte Induction from Nonhepatic Tissues and Its Clinical Use”
25 February 2002

Dr THIERRY, Annette
Institute Charles Sadron, CNES, France
“Heterogeneous Nucleation of Polyolefins by Organic Crystals:
Importance of Topological Rules”
4 June 2002

Prof WATANABE, Junji
Tokyo Institute of Technology, Tokyo, Japan
“Phase Transition of Block Copolymer with Liquid Crystalline
Polymer Chains”
17 June 2002

Dr WHEELLOCK, Craig E.
Department of Entomology and Cancer Research Center,
University of California, Davis, USA
“Novel Tools for the Investigation of Carboxyesterase Inhibition
and Substrate Selectivity”
1 November 2002

Prof WHITE, James L.
University of Akron, Akron, USA
“Structural Development in Melt Spinning and Drawing
Polyolefins : Influence of Additives on Polymer Extrusion”
13 November 2002

Prof Dr WILLIG, Frank
Dept. SE4, Dynamics of Interfacial Reactions, Hahn-Meitner-
Institute, Berlin, Germany
“Hot Electron Dynamics in InP with Two Different Atomic
Surface Reconstructions”
16 August 2002

Dr WILLIS, Martin R.
School of Chemistry, University of Nottingham, Nottingham,
U.K.
“Organic Electroluminescence—The Control of Hole Injection
by Electrode Modification”
25 November 2002

Prof WIRTH, Thomas
Department of Chemistry, Cardiff University, Cardiff, United
Kingdom
“Memory of Chirality or Remembering Chirality? Challenge
from Selenium Chemistry”
3 August 2002

Assoc Prof YAMAO, Fumiaki
National Institute of Genetics, Japan
“Does Ubiquitin Control Chromatin Functions? -Genetic
Recombination and Ubiquitin”
26 April 2002

Dr YANAGI, Hisao
Department of Applied Chemistry, Kobe University, Japan
“Organic Electronics and Photonics Devices Based on Molecular
Nanotechnology”
5 March 2002

Prof YOSHINAGA, Kohji
Faculty of Engineering, Kyushu Institute of Technology,
Fukuoka, Japan
“Formation of Colloid Crystals by Polymer-Modified Silica

Particles in Organic Solvent and Their Immobilization by Radical
Polymerization”
26 March 2002

Dr YUMOTO, Noboru
National Institute of Advanced Industrial Science and Technology,
Osaka, Japan
“Development of Caged Peptides Serving as a Light Switch for
Controlling Cellular Functions”
9 September 2002

Mr YURI, Yosuke
Hiroshima University, Japan
“Beam Simulation for Phase Transition of Fast Ion Beam”
25 February 2002

Dr ZORN, Reiner
Jülich Forschungszentrum, Jülich, Germany
“Dynamics of Soft-matter in Confinements”
5 March 2002

MEETINGS AND SYMPOSIUMS

Grant-in-Aid for Creative Scientific Research, Collaboratory on Electron Correlations — Towards a New Research Network between Physics and Chemistry —

10-11 January 2002 (Kyoto)

“Towards a Collaboration between ICR and Neutron Scattering Group in KEK”

Organized by NAKAHARA, Masaru

ICRIS '02 (The Sixth International Symposium Organized by Institute for Chemical Research (ICR), Kyoto University) The Science and Technology of Polymer Assembly: The Global Strategy in 21st Century

31 January - 1 February 2002 (Kyoto)

I. Oral Presentations

Prof TIRRELL, M.

Departments of Chemical Engineering and of Materials,
University of California, Santa Barbara, USA

“Building Macromolecular Assemblies with Information Content”

Prof RYAN, A. J.

Department of Chemistry, University of Sheffield, UK

“Towards Molecular Machines: Chemically Induced Oscillations in a pH Responsive Hydrogel”

Prof KAJIYAMA, T.

Department of Chemical Science & Technology, Faculty of Engineering, Kyushu University, Japan

“Differences in Molecular Aggregation Structure and Thermal Properties at Surface and in Bulk of Polymeric Solids”

Prof OSAKI, K.

Institute for Chemical Research, Kyoto University, Japan

“Molecular Rheology, eh ?”

Prof KAWAGUCHI, M.

Department of Chemistry for Materials, Faculty of Engineering, Mie University, Japan

“Displacement of Polymeric Systems in Hele Shaw Cells”

Prof AMIS, E. J.

Polymer Division, National Institute of Standards and Technology, USA

“Applications of Combinatorial Methods for Investigations of Polymer Physics”

Prof KORNFIELD, J.

Department of Chemical Engineering, California Institute of Technology, USA

“Biomedical Hydrogels from Self-Assembly of Fluoroalkyl-Ended PEG: Phase Behavior, Rheology and Erosion Kinetics”

Prof WEGNER, G.

Max-Planck Institute for Polymer Research, Germany

“From Macromolecules to Macromolecular Assemblies and Nanocomposites”

Prof RICHTER, D.

Institute for Solid State Research, Research Center Juelich, Germany

“Wax Control by Self-Assembling Polymers”

Prof KAJI, K.

Institute for Chemical Research, Kyoto University, Japan

“What Happens Prior to Crystallization of Polymers”

Prof TANAKA, H.

Institute of Industrial Science, University of Tokyo, Japan

“Mechanism of Network Formation in Viscoelastic Phase Separation”

Prof HASHIMOTO, T.

Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, Japan

“Viscoelastic Effects on Early Stage Spinodal Decomposition in Polymer Solutions”

Prof MATYJASZEWSKI, K.

Carnegie Mellon University, Center for Macromolecular Engineering, USA

“Well-Defined Macromolecular Structures at Surfaces by Atom Transfer Radical Polymerization (ATRP)”

Prof AIDA, T.

Department of Chemistry and Biotechnology, Graduate School of Engineering, University of Tokyo, Japan

“Fabrication of Nanoscopic Functional Materials from Inorganic and Biological Approaches”

Prof HARADA, A.

Graduate School of Science, Osaka University, Japan

“Design and Construction of Supramolecular Polymers Using Host-Guest Interactions”

II. Posters

IKEDA, Y., KITADE, T., KOHJIYA, S., HAYASHI, A., MATSUDA, A., TATSUMISAGO, M., MINAMI, T.

“Lithium Ion Conducting Glass-polymer Composites”

BEDIA, E. L., MURAKAMI, S., KOHJIYA, S.

“Structure and Properties of i-PP/EH Blends Under Uniaxial Drawing”

URAYAMA, K., YOKOYAMA, K., KOHJIYA, S.

“Viscoelastic Relaxation of End-linked Polydimethylsiloxane Networks Containing Unattached Linear Polydimethylsiloxane”

YOSHIOKA, T., TSUJI, M., KAWAHARA, Y., KIKUTANI, T., KOHJIYA, S.

“Structural Analysis of the High-speed Spun Polyester Fibers Using the Permanganic Etching Method”

USHINO, H., KONDO, K., KAWAGUCHI, A.

“Synthesis and Structure of Polyacetylene with Phenyleneethynylene Side Groups: $[-(\text{C}_6\text{H}_4-\text{C}\equiv\text{C})_n-\text{Si}(\text{iPr})_3]_n$; $n=1,2$ ”

TAGUCHI, K., MIYAJI, H., IZUMI, K., HOSHINO, A., MIYAMOTO, Y., KOKAWA, R.
“Effect of Thickness on Crystal Growth in Ultrathin Isotactic Polystyrene Films”

MIYAMOTO, Y., YAMAO, H., SEKIMOTO, K.
“Glass Transition and Deformation in Crosslinked Rubber”

INOUE, T., OSAKI, K.
“The Molecular Rheology: Polymer Dynamics in Solutions and Melts”

WATANABE, H., MATSUMIYA, Y., KANAYA, T., TAKAHASHI, Y.
“Rheology and Structure of Diblock Copolymer Micellar Lattice: Role of Concentration Fluctuation in Lattice Disruption”

SHIKATA, T., ITATANI, S.
“Rheology of Aqueous Threadlike Micellar Systems of Amine Oxide Type Surfactants”

NAKAMURA, Y., AMITANI, K., TERAOKA, K., NORISUYE, T.
“Small-angle X-ray Scattering from Polystyrene Polymacromonomers in Dilute Solution”

ASHIDA, Y., SATO, T., MORINO, K., MAEDA, K., YASHIMA, E., OKAMOTO, Y.
“Effect of Complexation with an Optically Active Amine on the Helical Conformation of Poly((4-carboxyphenyl)acetylene) in Dimethylsulfoxide”

SAKURAI, S., ISOBE, D., KOTA, T., OKAMOTO, S., YAO, T., NOMURA, S.
“Rupture of Gyroid Upon Uniaxial Stretching in a Microphase-separated SBS Triblock Copolymer”

NISHIDA, K., TAKEDA, T., KANAYA, T., KAJI, K.
“Phase Diagram of Polyelectrolyte Solutions - Added Salt Effects -”

TAKAHASHI, N., TAKESHITA, H., KANAYA, T., NISHIDA, K., KAJI, K.
“Observation of Speckle During Gelation Process of Poly(vinyl alcohol)”

KANAYA, T., MONKENBUSCH, M., WATANABE, H., NAGAO, M., RICHTER, D., KAJI, K.
“Dynamics of Polymer Micelles Studied by Neutron Spin Echo Technique - Breathing Mode or Zimm Mode ? -”

KAWAGUCHI, T., IDE, S., KANEKO, F.
“Structure and Morphology of Poly(*p*-dioxanone)”

TAKESHITA, H., KAWAGUCHI, H., NAGAI, M., ISHII, N., MIYA, M., TAKENAKA, K., SHIOMI, T.
“Crystallization Behavior and Structure Formation of Block Copolymers”

MURAKAMI, M., ISHIDA, H., HORII, F., YAMAMOTO, T.
“Structure and Structural Changes of a Main-chain Thermotropic Liquid Crystalline Polyether”

TSUNASHIMA, Y., KAWANISHI, H., HATTORI, K., MIZUNO, M., ONODERA, G., HORII, F.
“Dynamic Assemblies of Cellulose Acetates in Polar Solvents”

KAJI, H., HORII, F.
“Characterization of Specific Interactions in Polymers by an MAS NMR Method Without Irradiating Passive Spins”

HIRAI, A., TSUJI, M., HORII, F.
“Structure of Band-like Cellulose Assemblies Produced by *Acetobacter xylinum* as Revealed by TEM and X-ray Diffraction Analysis”

KIMURA, T.
“Magnetic Processing of Polymeric Materials”

GOTO, A., YOSHIKAWA, C., FUKUDA, T.
“Quantitative Comparison of Kinetic Theory and Experiment on Living Radical Polymerizations”

YAMAMOTO, S., EJAZ, M., TSUJII, Y., FUKUDA, T.
“Elevated Glass Transition Temperature of High-density Polymer Brushes”

OHNO, K., WONG, B., HADDLETON, D. M.
“Living Radical Polymerization with Oligosaccharide-based Initiators”

AOKI, H., ANRYU, M., KUNAI, Y., ITO, S.
“Two-D Imensional Phase-separation of Polymer Monolayer Studied by Scanning Near-field Optical Microscopy”

OKAMURA, H., TAKATORI, Y., TSUNOOKA, M., SHIRAI, M.
“Synthesis of Random and Block Copolymers of Styrene and Styrenesulfonic Acid with Low Polydispersity Using Nitroxide-mediated Living Radical Polymerization Technique”

TAKADA, A., RAHMAN, S. A., NEMOTO, N.
“Viscoelasticity of Potassium Neutralized Telechelic Poly(ethylene butylene) Ionomer Solutions in Non-polar Solvent”

17th International Colloquium on Magnetic Films and Surfaces (ICMFS 2002)
Organized by: Institute for Chemical Research, Kyoto University and COE of Elements Science, Kyoto University

Chair: SHINJO, Teruya

5-8 March 2002 (Kyoto)

PRISM Workshop: Phase Rotation Intense Slow Muons

22-23 March 2002 (Kyoto)

Mori, Y.
“Proton Driver / 100 Bunch Extraction”

Yoshimura, K.
“Target”

Nosaka, N.
“Pi Capture Simulation on PRISM”

Yokoi, T.
“FODO & FFAG Transport”

Morita, A.
“Helical Q Transport”

Iwashita, Y.
“PRISM/L Alternative ”

Yoshimura, K.
“Location of the Facility”

Onishi, H.
“Superconducting Magnet”

Sato, A.
“Phase Rotator”

Aiba, M.
“Acceptance of FFAG Phase Rotator”

Uesugi, T.
“RF Cavity for FFAG”

Widmann, E.
“A Possible Antiproton Facility at JHF “

Kitano, R.
“mu-e Conversion”

Sasao, N.
“μ-e Conversion Experiment with a Spiral Solenoid Spectrometer”

Takubo, T.
“R&D on Electron Trackers”

Kubo, K.
“Mossbauer Spectroscopy with Negative Muon Capture Reactions”

Sakamoto, S.
“DREAMX - New Tool for History Study with Muons -”

Ishida, K.
“Muon Catalyzed Fusion”

Discussion Meeting on “Structure Formation Mechanisms in Polymer Crystallization”

Chairperson: MIYAJI, Hideki (Kyoto University),
Secretary: KANAYA, Toshiji (Kyoto University)
14 June 2002 (ICR, Kyoto)

Prof KAJI, Keisuke
Kyoto University
“Details of Structure Formation During the Induction Period of Spinodal Type Polymer Crystallization”

Prof OLMSTED, Peter D.
University of Leeds
“What is the Role of the Melt Liquid Structure in Primary Polymer Crystallization?”

Prof STROBL, Gert
Universität Freiburg
“Polymer Melt Crystallization: Evidence for a Multi-Stage”

Prof MUTHUKUMAR, Murugappan
University of Massachusetts
“Chain Entropy and Primordial Stages of Polymer Crystallization from Solutions”

Prof BASSET, David Clifford
University of Reading
“New Aspects of The Influence of Lamellar Surfaces on Crystalline Polymers”

Prof TODA, Akihiko
Hiroshima University
“Twisting Correlation of Crystallites in Banded (Polymer) Spherulites”

Prof CHENG, Stephen Z. D.
The University of Akron
“Tailoring Polymer Crystalline Morphologies in Nano-templates of Self-assembled Block Copolymers”

Prof LOTZ, Bernard
Institute Charles Sadron
“Climbing the Ladder of Length Scales: Linking the Higher Order Structure of Crystalline Polymers and Their Molecular Organization”

Microbial Polymers Symposium

Organized by HORII, Fumitaka
26-27 July 2002 (ICR)

Group Meeting: Grant-in-Aid for Creative Scientific Research, Collaboratory on Electron Correlations — Towards a New Research Network between Physics and Chemistry — , 2nd Group

Organized by NAKAHARA, Masaru
2-3 August 2002 (Kyoto)

Symposium on “Recent Topics in Dark Matter Search”

Organized by MATSUKI, Seishi and MASAIKE, Akira
7 August 2002 (International Institute for Advanced Studies, Kyoto)

ISPA (International Seminar on Photoionization in Atom by Institute for Chemical Research (ICR), Kyoto University)

19-20 August 2002 (Kyoto)

I. Oral Presentations

Prof HAMMOND, P.
Department of Physics, University of Western Australia, Australia
“Uncovering Doubly Excited States by Fluorescence”

Dr HARRIES, J.
Department of Physics, Queen’s University Belfast, England
“Helium Double Photo-excitation in a Strong Electric Field”

Prof RUBENSSON, J. -E.
Department of Physics, Uppsala University, Sweden
“External Field Effects on the Doubly Excited States of Helium”

Dr FANG, T. -K.
Department of Physics, Fu Jen Catholic University, Taiwan
“B-spline-based Complex-rotation Method for Two-electron and Divalent Atoms”

Prof GORCZYCA, T.
Department of Physics, Western Michigan University, USA
“Radiative, Relativistic and Electric Field Effects on Doubly-excited State of Helium”

Prof AMUSIA, M.
Racah Institute, Hebrew University, Israel
“Correlation Effects at High Photon Energies”

Dr MORISHITA, T.
Department of Physics, University of Electro-Communications, Japan
“Visualization of Electron Correlations in Triply Excited States of Atoms”

Prof KOIKE, F.
Center of Scientific Information, Kitasato University, Japan
“Survey of Hollow Atomic States and Their Dynamics”

Prof DEUTSCH, M.
Department of Physics, Bar-Ilan University, Israel
“The Evolution of Multielectronic X-Ray Spectra from Threshold to Saturation”

Prof STEFANI, G.
Department of Physics, Università di Rome Tre, Italy
“Inner Shell Ionization Dynamics Studied by Electron Electron Coincidence Experiments”

Prof BERRA, N.
Department of Physics, Western Michigan University, USA
“K-shell Photodetachment of Negative Ions”

Prof PEGG, D.
Department of Physics, University of Tennessee, USA
“Correlated Processes in Photodetachment”

Prof KRAISOV, V.
Physics Division, Moscow Institute of Physics and Technology, Russia
“Barrier-suppression Ionization of Complex Atoms by Super-intensity Laser Fields”

Prof SHERMANN, E.
Physics Division, Moscow Institute of Physics and Technology, Russia
“Inelastic X-ray Scattering in Solids: a Bridge to Low-energy Excitations”

Dr HEBERT, C.
Department of Physics, Technical University of Wien, Austria
“Theory of Core-loss Spectroscopies - Comparison of ELNES with XANES”

Prof DOUSSE, J. -CL.
Department of Physics, University of Fribourg, Switzerland
“2s and 3s Atomic Level Widths of Mid-heavy and Heavy elements”

Dr OURA, M.
Harima Institute, RIKEN, Japan
“Near Threshold Evolution of Multielectron Processes in Photoionization”

Dr VLAICU, A. M.
BL15XU Spring-8, National Institute for Material Science, Japan
“Photo-excitation of Multi-electron Transitions in Heavy Elements by Synchrotron Radiation”

II. Posters

ITO, Y., TOCHIO, T., SHIGEOKA, N., OOHASHI, H., VLAICU, A. M., KANEYOSHI, T., MOTOYAMA, M., SHOJI, T., FUKUSHIMA, S.

“A Trial Fitting on $K\alpha_{1,2}$ Emission Spectra in Transition Elements”

KABACHNIK, N. M., SAZHINA, I. P.
“Relations between Intrinsic Spin Polarization Parameters for Auger Electrons”

SHIGEOKA, N., OOHASHI, H., ITO, Y., TOCHIO, T., VLAICU, A. M., NISAWA, A., YOSHIKAWA, H., FUKUSHIMA, S., WATANABE, M.
“The Behavior of Fe $K\alpha$ Satellites around the Threshold”

OOHASHI, H., SHIGEOKA, N., TOCHIO, T., ITO, Y., VLAICU, A. M., NISAWA, A., YOSHIKAWA, H., FUKUSHIMA, S., WATANABE, M.
“The Contribution of the Indirect Ionization to Au $L\beta_2$ Satellites”

KAWATSURA, K., TAKAHIRO, K., MORIKAWA, T., MURAMATSU, Y., PERERA, R. C. C.
“Excitation-energy Dependence of Cu $L_{2,3}$ X-ray Emission Spectra of Cu, Cu₂O and CuO”

LAMBOURNE, J., LALANQUIE, P., HALL, R. I., AHMAD, M., ZITNIK, M., BUCAR, K., STRANGES, S., HAMMOND, P., PENENT, F.
“Exploration of Doubly Photo-excited Helium Triplet States via the Study of Metastable Atom Yield and Fluorescence Angular Distributions”

FUKUSHIMA, S., YOSHIKAWA, H., KIMURA, M., TANAKA, A., VLAICU, A. M., KITA, Y., WATANABE, K., NISAWA, A., YAGI, N., OKUI, M., TAGUCHI, M., OIWA, R.
“The Observation of the Cascade Auger Process by Threshold Excitation”

KJELDSSEN, H., FOLKMANN, F., HANSEN, J., WEST, J.,
“Photoionization of the Singly-charged Ions of the Transition Elements”

POONIA, S.,
“ $L\beta_1$ Satellites in X-ray Emission Spectra of ^{41}Nb , ^{45}Rh , ^{47}Ag and ^{49}In Elements”

UEDA, K.,
“Interference Effects in the Resonant Photoemission Channels to the $\text{Ne}^+ 2p4(^1D_2) 3p\ ^2P, ^2D$, and 2F States in the Ne 1s Excitation Region”

UEDA, K.,
“Evolution from Resonant to Normal Auger Spectra across the Ne 1s Threshold”

The 1st Symposium on Composite Biocatalysts

Organized by Esaki, Nobuyoshi
Nine subjects were presented

18 October 2002 (Kyoto)

7th Symposium on Power Supply Technology for Accelerator

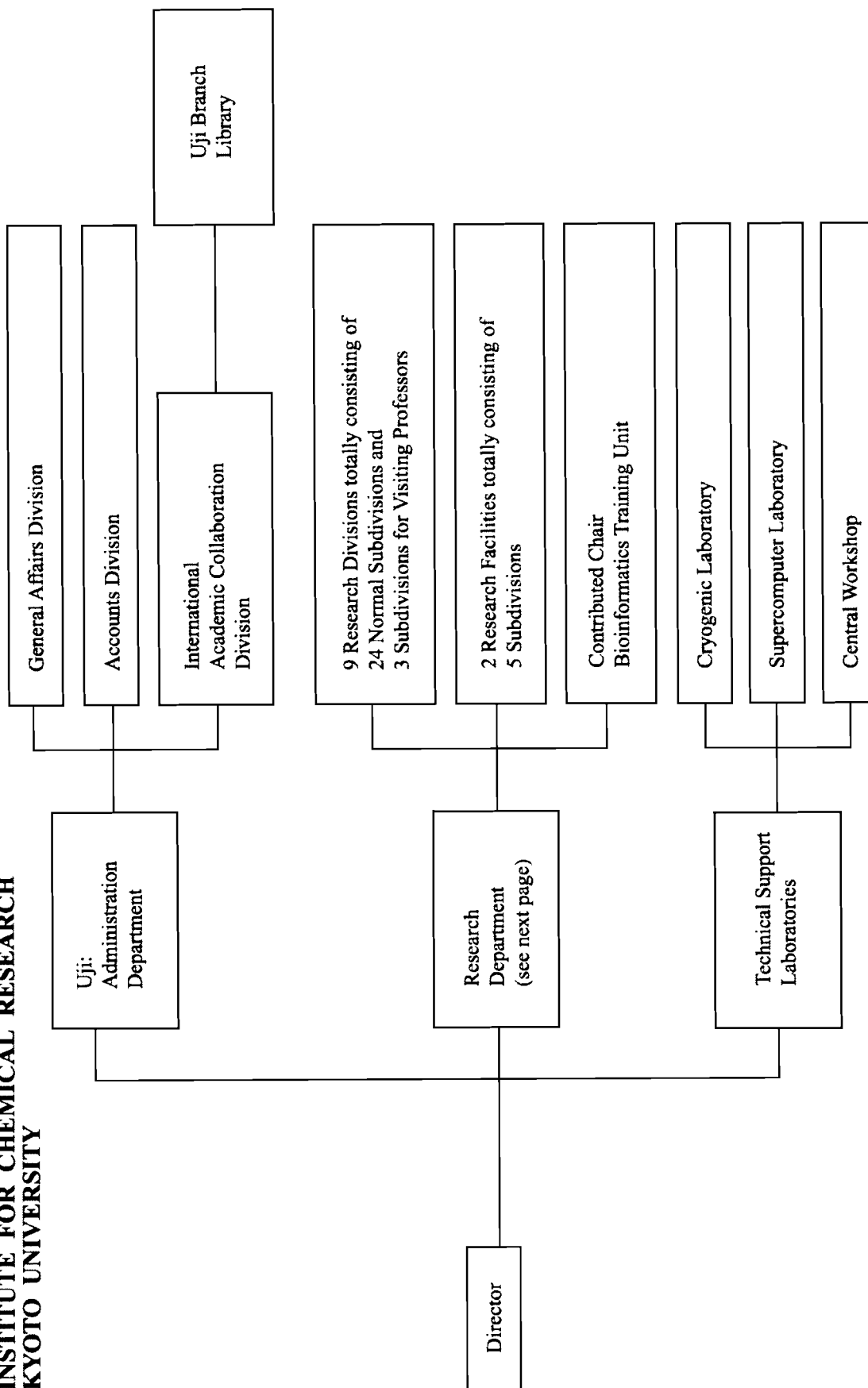
Organized by SHIRAI, Toshiyuki; IWASHITA, Yoshihisa;
NODA, Akira
Nineteen subjects were presented

12-13 December 2002 (Shirahama, Japan)



ORGANIZATION AND STAFF

INSTITUTE FOR CHEMICAL RESEARCH KYOTO UNIVERSITY



INSTITUTE FOR CHEMICAL RESEARCH, KYOTO UNIVERSITY (As of 31 December 2002)
RESEARCH DIVISION (G: Laboratory for Visiting Professors)

Research Division	Subdivision (Laboratory)	Professor	Associate Professor	Instructor	Technician
Director TAKANO, Mikio	States and Structures				
	I. Atomic and Molecular Physics	HATA, Yasuo	ITO, Yoshiaki	NAKAMATSU, Hirohide	
	II. Electron Microscopy and Crystal Chemistry	ISODA, Seiji	KURATA, Hiroki	OGAWA, Tetsuya NEMOTO, Takashi	MORIGUCHI, Sakumi
Interface Science	III. Polymer Condensed States	KOHJIYA, Shinzo	TSUJI, Masaki	URAYAMA, Kenji TOSAKA, Masatoshi	
	I. Solutions and Interfaces	NAKAHARA, Masaru	UMEMURA, Junzo	MATSUMOTO, Mutsuo MATUBAYASHI, Nobuyuki	WAKAI, Chihiro
	II. Molecular Aggregates	SATO, Naoki	ASAMI, Koji	OKAMURA, Emiko KITA, Yasuo	
Solid State Chemistry	III. Hydrospheric Environment Analysis	SOHRIN, Yoshiki	UMETANI, Shigeo	YOSHIDA, Hiroyuki SASAKI, Yoshihiro	NORISUYE, Kazuhiro
	I. Artificial Lattice Alloys			OKAMURA, Kei FUJITA, Masaki	MINAMI, Tomoharu
	II. Quantum Spin Fluids	YAMADA, Kazuyoshi		IKEDA, Yasunori	KUSUDA, Toshiyuki
Fundamental Material Properties	III. Solid State Chemistry	TAKANO, Mikio	TERASHIMA, Takahito	AZUMA, Masaki	
	IV. Amorphous Materials	YOKO, Toshinobu		TAKAHASHI, Masahide SHIMADA, Ryoko	DORJPALAM, Enkhvuvshin
Organic Materials Chemistry	G. Structure Analysis	KANNO, Ryoji	MITANI, Seiji		
	I. Molecular Rheology		WATANABE, Hiroshi	INOUE, Tadashi	OKADA, Shinichi
	II. Polymer Materials Science		KANAYA, Toshiiji	NISHIDA, Koji	
Synthetic Organic Chemistry	III. Molecular Dynamic Characteristics	HORI, Fumitaka	TSUNASHIMA, Yoshitsuke	KAJI, Hironori HIRAI, Asako	OHMINE, Kyoko
	G. Composite Material Properties	YAMAMOTO, Yasushi	SAITO, Hiromu		
	I. Polymeric Materials	FUKUDA, Takeshi	TSUJII, Yoshinobu	MURAKAMI, Syozo OHNO, Kotiji	
Bioorganic Chemistry	II. Organic Structural Chemistry	KOMATSU, Koichi	KITAGAWA, Toshikazu	GOTO, Atsushi NISHINAGA, Tohru	
	I. Synthetic Design	TAMAO, Kohei		MURATA, Yasujiro YAMAGUCHI, Shigehiro	
	II. Fine Organic Synthesis		KAWABATA, Takeo	TSUJI, Hayato	TERADA, Tomoko
Molecular Biofunction	G. Synthetic Theory	NAKA, Takehiko	SUGIHARA, Takumichi	TSUBAKI, Kazunori	
	I. Organoclement Chemistry	TOKITOH, Norihiro	NAKAMURA, Kaoru	SUGIYAMA, Takashi KAWAI, Yasushi	YAMAZAKI, Norimasa HIRANO, Toshiko
	II. Bioactive Chemistry	SUGIURA, Yukio	FUTAKI, Shiroh	TAKEEDA, Nobuhiro	
Molecular Biology and Information	III. Molecular Clinical Chemistry	UEDA, Kunihiko	TANAKA, Seigo	NAGAOKA, Makoto	
	I. Chemistry of Molecular Biocatalysts	SAKATA, Kanzo	HIRATAKE, Jun	MIZUTANI, Masaharu SHIMIZU, Bun-ichi	
	II. Molecular Microbial Science	ESAKI, Nobuyoshi	YOSHIMURA, Tohru	KURIHARA, Tatsuo MIHARA, Hisaaki	
Bioinformatics Center	I. Biopolymer Structure			HIRAGI, Yuzuru FUJII, Tomomi	
	II. Molecular Biology	OKA, Atsuhiko	SUGISAKI, Hiroyuki AOYAMA, Takashi	SAKAI, Hiroe	YASUDA, Keiko
	I. Bioknowledge Systems	KANEHISA, Minoru	GOTO, Susumu	NAKAYA, Akihiro KAWASHIMA, Shuichi	
Contributed Chair Bioinformatics Center	II. Biological Information Network	AKUTSU, Tatsuya		OKUNO, Yasushi UEDA, Nobuhisa	
	III. Pathway Engineering	MIYANO, Satoru			
	Proteome Informatics (SGI JAPAN)	TOH, Hiroyuki	MAMITSUKA, Hiroshi	YAMAGUCHI, Atsuko	
Nuclear Science Research Facility	Bioinformatics Training Unit		KUMA, Keiichi	DAIYASU, Hiromi ICHIHARA, Hisako	TONGU, Hiromu
	I. Particle and Photon Beams	NODA, Akira	IWASHITA, Yoshihisa	SHIRAI, Toshiyuki	
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