Preface

The history of the Institute for Chemical Research (ICR) dates back to 1915, when a specialized Center was established within Kyoto University. This Center conducted research and production of Salvarsan and other pharmaceutical products, and laid the base for the ICR. The ICR was formally established in 1926 with the founding philosophy of “Conducting Fundamental Studies and Exploring Their Application to Special Fields of Chemistry”. The present ICR consists of five major Research Divisions and three affiliated centers, where a total of 106 full-time faculty members and 230 graduate students form the 36 laboratories (5 of which are guest laboratories).

The ICR is extremely active in a wide range of research fields covering chemistry, physics, biology, and informatics. Many members of our staff have participated in major national projects such as the 21st Century COE (Center of Excellence) Program and also in commissioned researches, that have generated outstanding results in advanced research fields.

At the ICR we have also made extensive contributions to education. Each laboratory is affiliated with one of the Graduate Schools including Science, Engineering, Agriculture, Pharmaceutical Sciences, Medicine, Informatics, and Human and Environmental Studies of Kyoto University. The high standard of degree we award at the ICR every year represents our devotion in the field of professional education. At the same time, we provide the public with opportunities to visit the ICR by holding lectures and tours on a regular basis.

April 1, 2004, saw the birth of the “National University Corporation, Kyoto University”, a change enabling Kyoto University to explore more independence in its administration. ICR has taken this change one step further to create an environment with even more active research motivation. We reorganized the ICR to the present system and improved the mobility of our staff by implementing a tenure track system. We will further invest our energy to strengthen our “social contributions” based on the concept of “Science in society and science for society” (a proclaim made at the 1999 World Conference on Science and the Use of Scientific Knowledge). Of course, this should go hand in hand with the idea of “science for the sake of science”. We encourage young researchers to challenge their interdisciplinary boundaries at the ICR, the great melting pot, to form inspiring concepts leading to great discoveries.

We invite you to look into our recent achievements and the scope of our future.

January 2005

Mikio Takano
Director
ICR News 2004

“Challenge and Innovation”
Reorganization of the Institute for Chemical Research

The Institute for Chemical Research was reorganized in 2004 to five Research Divisions and three Research Centers.

Division of Environmental Chemistry
This research group aims to contribute to the development of a sustainable society through fundamental studies such as structural characterization and dynamics of solutions and polymers, in particular under extreme conditions, biochemistry in the hydrothermal, and biotechnology with useful enzymes and microorganisms.

Division of Biochemistry
Biology meets Chemistry; elucidating the mechanisms behind intra-cellular organelle organization, stimuli response, and biomolecular synthesis in living matters for pioneering novel materials.

Division of Synthetic Chemistry
Research is conducted for creation of “Novel Materials” from viewpoints irrespective of disciplines of organic and inorganic chemistry and for clarification of their structures, functions, and properties.

International Research Center for Elements Science
Proposal of a guideline for creation of novel elementary materials through the uncovering of rule of key elements which determine the functions of materials.

Division of Materials Chemistry
Emphasizing hybridization and/or composite-preparation from incompatible combinations, creation of novel functionality materials is aimed.

Division of Multidisciplinary Chemistry
By exploring viewpoints aiming at merging science with engineering, we are going to upgrade the paradigm of our research in the boundary region among chemistry, physics and biology. In cooperation with other divisions and centers in our institute, we will develop exploratory basic researches for fostering advanced materials science.

Bioinformatics Center
Our laboratory promotes research in bioinformatics and the development of the foundation for an integrated and extensive resource for the Bioscience.

Advanced Research Center for Beam Science

Basic Research for the Development of Science and Technology
Material Control for the Development of Society
The Establishment of
“Advanced Research Center for Beam Science”

In order to organize the interdisciplinary research among different individual scientific researches related with beams, the Advanced Research Center for Beam Science has been started from April 1, 2004 combining Nuclear Science Research Facility with two laboratories of “Atomic and Molecular Physics” and “Electron Microscopy and Crystal Chemistry”. The center is composed of the four laboratories oriented for Particle Beam Science, Laser Matter Interaction Science, Electron Microscopy and Crystal Chemistry and Structural Molecular Biology. The role of the center is not only stimulating the collaborations among these laboratories but also to initiate the collaborations with the outside groups both in and out of our institute.

On 24 April 2004, the opening of the center was celebrated with the talks given by Prof. Bunzo Tsuji, Vice President of Kyoto University, Prof. Noboru Sasaki, Dean of the Graduate Course of Science, Prof. Hiroyuki Tomita, Dean of Graduate School of Human and Environmental Studies, Dr. Satoru Yamada, Director of Department of Accelerator Physics and Engineering, National Institute of Radiological Sciences, and Prof. Igor Meshkov, Director of Science, Joint Institute for Nuclear Research, Dubna and Member of Academy of Science, Russia.

The Opening Ceremony of the Advanced Research Center for Beam Science, 24 April 2004.

http://sun.sci.kyoto-u.ac.jp/~sakabe/ARBS-Home.html
CONTENTS

Preface ......................................................................................................................... iii

ICR News 2004 ............................................................................................................. iv

ORGANIZATION .......................................................................................................... 1

TOPICS AND IntroDUCTORY COLUMNs OF LABORATORIES ................................. 3
  Division of Synthetic Chemistry
    Organoelement Chemistry .................................................................................. 4
    Structural Organic Chemistry ........................................................................... 6
    Synthetic Organic Chemistry .......................................................................... 8
    Advanced Inorganic Synthesis ....................................................................... 10

  Division of Materials Chemistry
    Chemistry of Polymer Materials ...................................................................... 12
    Chemistry of Polymeric Functionality Materials ........................................ 14
    Inorganic Photonics Materials ......................................................................... 16
    Magnetic Materials ........................................................................................ 18

  Division of Biochemistry
    Biofunctional Design-Chemistry ...................................................................... 20
    Chemistry of Molecular Biocatalysts ............................................................ 22
    Molecular Biology .......................................................................................... 24
    Molecular Clinical Chemistry ......................................................................... 26

  Division of Environmental Chemistry
    Molecular Materials Chemistry ........................................................................ 28
    Hydrospheric Environment Analytical Chemistry ......................................... 30
    Solution and Interface Chemistry .................................................................. 32
    Molecular Microbial Science ........................................................................ 34

  Division of Multidisciplinary Chemistry
    Polymer Materials Science ............................................................................. 36
    Molecular Rheology ......................................................................................... 38
    Molecular Aggregation Analysis ..................................................................... 40
    Supramolecular Biology ................................................................................ 42

  Advanced Research Center for Beam Science
    Particle Beam Science ........................................................................................ 44
    Laser Matter Interaction Science .................................................................... 46
    Electron Microscopy and Crystal Chemistry ................................................ 48
    Structural Molecular Biology .......................................................................... 50
International Research Center for Elements Science

Organic Main Group Chemistry ................................................................. 52
Advanced Solid State Chemistry ............................................................... 54
Organotransition Metal Chemistry ............................................................. 56
Photonic Elements Science .................................................................... 58

Bioinformatics Center

Bioknowledge Systems ............................................................................ 60
Biological Information Network ................................................................. 62

Contributed Chair

Proteome Informatics (SGI Japan) ............................................................. 64

Bioinformatics Center

Bioinformatics Training Unit ...................................................................... 66

VISITING PROFESSORS’ ACTIVITIES IN ICR .............................................. 69

PERSONAL .................................................................................................. 73
Retirement ................................................................................................. 74
Early Retirement ....................................................................................... 76
Awards ...................................................................................................... 77
Paper Awards ............................................................................................ 80
Poster Awards ........................................................................................... 81
Obituary .................................................................................................... 83

PUBLICATIONS .......................................................................................... 88

INTERNATIONAL RESEARCH COLLABORATIONS .................................. 105

THESSES .................................................................................................. 106

THE 104TH ICR ANNUAL SYMPOSIUM .................................................. 110

SEMINARS .................................................................................................. 114

MEETINGS AND SYMPOSIAUNMS .......................................................... 118

INDEX ....................................................................................................... 123
NAME INDEX ............................................................................................ 124
KEYWORD INDEX ..................................................................................... 127
**Abbreviations used in the columns**

<table>
<thead>
<tr>
<th>Term</th>
<th>Full Name</th>
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<td>D Pharm Sc</td>
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<td>Post-Doctoral Research Fellow</td>
<td>Ph D</td>
<td>Doctor of Philosophy</td>
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ORGANIZATION
5 Divisions and 3 Centers

- Division of Synthetic Chemistry
  - Organoelement Chemistry
  - Structural Organic Chemistry
  - Synthetic Organic Chemistry
  - Advanced Inorganic Synthesis
- Division of Materials Chemistry
  - Chemistry of Polymer Materials
  - Chemistry of Polymeric Functionality Materials
  - Inorganic Photonics Materials
  - Magnetic Materials
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  - Chemistry of Molecular Biocatalysts
  - Molecular Biology
  - Molecular Clinical Chemistry
- Division of Environmental Chemistry
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  - Solution and Interface Chemistry
  - Molecular Microbial Science
- Division of Multidisciplinary Chemistry
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  - Molecular Rheology
  - Molecular Aggregation Analysis
  - Supramolecular Biology

Laboratories

- Advanced Research Center for Beam Science
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  - Laser Matter Interaction Science
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  - Organic Main Group Chemistry
  - Advanced Solid State Chemistry
  - Organotransition Metal Chemistry
  - Photonic Elements Science
- Bioinformatics Center
  - Bioknowledge Systems
  - Biological Information Network
  - Pathway Engineering
  - Proteome Informatics (SGI Japan)
  - Genome Informatics

Research Divisions

- Research Centers
- Contributed Chair
- Bioinformatics Training Unit
- Visiting Divisions
- Supercomputer Laboratory
- Low Temperature Laboratory
- Central Workshop

(Institute for Chemical Research)

(Reorganized on April 2004)
TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES
Division of Synthetic Chemistry
- Organoelment Chemistry -

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

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Scope of Research

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

Research Activities (Year 2004)

Presentations


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


Tokito N, Synthesis of metallasalicyclop benzences derivatives by using bulky substituents and the elucidation of their properties, Grant-in-Aid for Exploratory Research, 1
Synthesis of the First Stable Ferrocenyl-diphosphene and Elucidation of its Redox Behavior

A number of examples of kinetically stabilized diphosphenes (RP=PR), and diaranes (RSA=AsR) have been isolated and characterized. In addition, we have reported the synthesis of novel doubly bonded systems between heavier group 15 elements, i.e., disthene (RSb=SbR), dibismuthene (RBi=BiR), etc. by taking advantage of efficient steric protection groups, Tbt and Bbt groups. Recently, much attention has been paid to redox-active species containing a diphosphene unit in the field of molecular electronics and switches. Although generation of a ferrocenyl diphosphene, Mes*-P=PfC (Fc = ferrocenyl, Mes* = 2,4,6-tri-t-butylphenyl), has been reported by Pietschnig and Niecke, detailed studies have not been fully accomplished due to its instability in solution. Recently, we succeeded in the synthesis of a new ferrocenyl diphosphene Tbt-P=PfC and revealed its unique multi-switchable electrochemical properties.

Diphosphene I was synthesized by the dehydrochlorination reaction of Tbt–P(H)–P(Cl)–Fc with DBU. In sharp contrast to Mes*-P=PfC, I is very stable in the solid state and even in solution. The molecular structure of I was confirmed by NMR spectra and X-ray crystallographic analysis, which evidenced the P=P double-bond character of I. The cyclic voltammograms of I showed the reversible reduction and oxidation couples at -1.91 and +0.34 V vs. SCE, respectively. The electrochemical results for I were reasonably supported by the DFT calculations, which suggested that the LUMO and HOMO orbitals should be mainly π* orbital of the diphosphene moiety and d orbitals of the iron(II) atom, respectively.

Unprecedented Insertion Reaction of a Silylene into a B-B Bond and Generation of a Novel Borylsilyl Anion

Borylsilyl anions, i.e., silicon analogues of boron-stabilized carbanions, have been completely unprecedented species. We have recently developed a novel synthetic method for silylboranes derivatives based on the unique insertion reactions of an overcrowded silylene 2 [Tbt(Mes/Si)] into B–X (X = H or halogen) bonds. In addition, the synthesis of a diborylsilane, Tbt[Mes/Si][B(pin)]= [3, pin = pinacolato] was achieved via the insertion reaction of 2 with bis(pinacolato)boron. These reactions are quite important from the standpoints of development on a new synthetic method for borylsilanes and elucidation of reactivities of silylenes. Furthermore, the reaction of 3 with n-BuLi resulted in the generation of borylsilyl anion 4, which could be trapped by chlorotrimethylsilane. It is noteworthy that the formation of 4 is the first example for the generation of a borylsilyl anion and that a diborylsilane is shown to be a possible precursor for a borylsilyl anion.
Division of Synthetic Chemistry
- Structural Organic Chemistry -

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

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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 α-π interaction; synthesis of new redox-active and supramolecular π-systems; organochemical transformation of fullerenes C_{60} and C_{70}, specifically the synthesis of open-cage fullerene derivatives and introduction and encapsulation of small molecules in the fullerene cage; generation of alkylated C_{60} and C_{70} cations and their application for the synthesis of functional materials.

Research Activities (Year 2004)

Presentations
Organic Functionalization of C_{60} Toward Synthesis of Endohedral Fullerene, Komatsu K, Murata Y, Murata M, The 205th Meeting of The Electrochemical Society, 12 May, San Antonio, USA.


Grants

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

A cyclopentadienyl radical, incorporating annelated two homoadamantene frameworks and a tert-butyl group, was synthesized and isolated in stable, crystalline form by the single electron oxidation of the corresponding cyclopentadienyl amion with silver ion [1]. The X-ray structure clearly demonstrated distinct bond alternation in the cyclopentadienyl ring, suggesting that radical 1 has the characteristics of a spin-localized 2,4-cyclopentadienyl-1-yl radical. The two homoadamantene frameworks are nonequivalent in crystals at 100 K, while ESR spectra indicated that they are equivalent in toluene at room temperature due to rapid changes in conformation. These characteristics are fundamentally different from those previously reported for uniformly substituted cyclopentadienyl radicals, thus displaying the distinctive effect of annelation with rigid homoadamantene frameworks on the nature of cyclic π-conjugated systems.

A New π-Conjugated Silylum Ion

Novel cationic silaaromatics, 2-silaimidazolium cation 3 was synthesized by chloride abstraction from the corresponding chlorosilane 2 with [Et₃Si(benzene)]PPFB⁺ (PPFB⁺ = tetraakis(pentfluorophenyl)borate) [2]. Cation 3 exists as a free silylum ion in solution due to bulky substituents on the five-membered ring. NMR spectroscopy and theoretical calculations showed the presence of aromaticity in 2-silaimidazolium ring, although its extent is smaller than that of the carbon analogue. The combined electronic effects of 6-π aromaticity and C–Si hyperconjugation are effective for stabilization of cation 3.

Generation of Fullereny Cation

(EtO)₃P⁺(OH)CH₂-C₆₀

Fullerenes are typically electronegative molecules, and only a few examples are known for their cations. Nevertheless, a novel fullereny cation, (EtO)₃P⁺(OH)CH₂-C₆₀, was quantitatively generated by simply dissolving RC₆₀H or RC₆₀H-R (R = CH₃P(O)(OEt)₂) in H₂SO₄. The cation was also generated in CD₂Cl₂ by the reaction of RC₆₀H or RC₆₀H-R with (2,4-Br₂C₆H₃)₃N⁺SbF₆⁻. The red-colored cation has a structure having an extra proton on a phosphoryl oxygen with the cationic center coordinated by the protonated oxygen. Various nucleophiles add to the cation selectively at 2- or 4-position, providing a new way to functionalize fullerenes [3].

References


Awards


Division of Synthetic Chemistry
- Synthetic Organic Chemistry -

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

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Prof. KAGAN, Henri Boris

Department of Chemistry, University of Manchester, England, 26 March, 2004
Institut de Chimie Moléculaire et des Materiaux, Universite de Paris-Sud, France, 18 - 19 November, 2004

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 and nitrogen heterocycles, visualization of molecular chirality by functionalized phenolphthalein, use of homocuxalixarene for molecular recognition, and the structural and functional investigation of heterochiral oligomers.

Research Activities (Year 2004)

Presentations
Asymmetric Synthesis of Cyclic Amino Acids via Memory of Chirality, KAWABATA T, IUPAC International Conference on Biodiversity and Natural Products: Chemistry and Medicinal Applications, 31 January.
Asymmetric Synthesis of Cyclic Amino Acids via Enolates with Dynamic Chirality, KAWABATA T, 7th International Symposium on Carbanion Chemistry, 11 July.

Grants
Kawabata T, Asymmetric Cyclization based on the
A Novel Route to Highly Substituted Nitrogen Heterocycles from α-Amino Acids

Nitrogen-containing heterocycles constitute important pharmacophore for drug discovery, useful building blocks for natural product syntheses, and the key structural subunits in asymmetric catalysis. We developed a novel route to highly substituted nitrogen heterocycles from readily available α-amino acids. Treatment of 1 with potassium hexamethyldisilazide (KHMDS) at –78°C gave tetrahydroquinoline derivative 2 as a single diastereomer in 95% ee. Similarly, on treatment of 3 with KHMDS at 0°C gave indoline derivative 4 in 95% ee. Chirality of the parent amino acid derivatives was preserved during the enolate-formation and the subsequent conjugate addition process. Thus, asymmetric synthesis was accomplished in the absence of external chiral sources such as chiral catalysts. This method is applicable to the synthesis of various nitrogen heterocycles with contiguous quaternary and tertiary stereocenters.

Temperature-Dependent Visual Enantiomeric Recognition of β-Amino Alcohols

Optically active artificial host molecule 7 consisting of a phenolphthalein skeleton and two crown ethers has been prepared and used for visual enantiomeric recognition of β-amino alcohols in a protic media. A wide range of (S)-β-amino alcohols induced deeper coloration in 7 than the corresponding (R)-β-amino alcohols at 0°C. The absorbance inversion temperatures (AIT) were observed within the range of 0 to 50°C in the several cases. For example, the absorption between 7 and (S)-phenylglycinol is stronger than that with (R)-form below 19.9°C. On the other hand, color development with 7 and (R)-phenylglycinol is deeper above this temperature. This is one of the very few examples where AIT is observed in a diastereomeric host-guest interaction.


Awards
MONGUCHI Daiki, Best Poster Award, 21st Summer School of Synthetic Organic Chemistry, 14 July 2004.
Division of Synthetic Chemistry
- Advanced Inorganic Synthesis -

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

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Experimental Station, DuPont CR&D, USA, 26 October 2004

Scope of Research

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

Research Activities (Year 2004)

Presentations

New perovskite-type oxides with possibly large ferroelectric polarizations, Y. Shimakawa, S. Niitaka, A. A. Belik, M. Azuma, and M. Takano, 2004 Autumn ISAP annual meeting, Sendai, Japan, 1 September 2004.

Crystal and electronic structures, physical properties, and material degradations of ferroelectric oxides used for FeRAMs, Y. Shimakawa, Fourth International Conference on Inorganic Materials, Antwerp, Belgium, 19 September 2004.


Diverse magnetic properties among low-dimensional BaM$_2$O$_3$ (M = Co, Ni, and Cu) and BaCuV$_2$O$_7$, A.A. Belik, M. Azuma, and M. Takano, Fourth International Conference on Inorganic Materials, Antwerp, Belgium, 20 September 2004.


Grants

High-Pressure Synthesis of PbVO$_3$
- A New Member of PbTiO$_3$ Family -

Ferroelectricity in ionic crystals is closely related to distortions of the crystal structure since the atomic displacement is the origin of the electric polarization. PbTiO$_3$ is a well known ferroelectric with a large spontaneous polarization, $P_s$, of 81 $\mu$C/cm$^2$ at room temperature. Existence of the 6$s^2$ lone electron pair of Pb$^{2+}$ ion and the orbital hybridization between the Pb 6$s$ state and O 2$p$ states in PbTiO$_3$ play crucial roles for the large tetragonal distortion ($c/a = 1.06$ at RT, where $a$ and $c$ are the lattice parameters) and large $P_s$ among the related compounds, e.g., BaTiO$_3$.

![Figure 1. Crystal structure of PbVO$_3$ determined by means of synchrotron X-ray powder diffraction study. Heavy atomic displacements give rise to a large spontaneous polarization.](image1)

PbTiO$_3$ is the only simple perovskite oxide with the composition PbM$\text{O}_3$ ($M$ is a transition metal) which can be prepared at ambient pressure. We found that a new perovskite-type oxide PbVO$_3$, isotypic with PbTiO$_3$, can be obtained by high-pressure synthesis at 6 GPa. The tetragonal phase was stable up to the decomposition temperature of 570 K at ambient pressure while a transition to cubic phase took place at 2 GPa. The tetragonal distortion is the largest in PbVO$_3$ among the reported PbTiO$_3$-type materials that suggests a large polarization of PbVO$_3$.

A Designed New Ferromagnetic Ferroelectric Compound Bi$_2$NiMnO$_6$

Magnetic ferroelectrics attract much attention because of the possible application for the data storage device and the fascinating coupling between magnetism and dielectric properties. A classical way to obtain a magnetic ferroelectric is to combine Bi$^{3+}$ or Pb$^{2+}$ ions with magnetic transition metal ions in a perovskite structure so that the 6$s^2$ lone pair of Bi$^{3+}$ (Pb$^{2+}$) and the strong covalent character of Bi(Pb)-O bond stabilize a noncentrosymmetric distorted structure. A ferromagnetic insulator can be obtained by distributing 2 kinds of transition metal ions with and without $e_g$ electrons in a NaCl type configuration.

![Figure 2. Crystal structure (left) and the magnetic susceptibility data (right) of Bi$_2$NiMnO$_6$. NaCl type distribution of Ni$^{3+}$ and Mn$^{4+}$ ions is the origin of the ferromagnetism.](image2)

A designed ferromagnetic ferroelectric double provskite Bi$_2$NiMnO$_6$ was prepared by means of high-pressure synthesis. The noncentrosymmetric structure and the ordering of Ni$^{3+}$ and Mn$^{4+}$ were confirmed by synchrotron X-ray powder diffraction study. The bulk sample showed ferroelectric and ferromagnetic transitions at 485 and 140 K, respectively. This simple material design should be applied to other Bi$_2M^{3+}M'^{4+}$O$_6$ and Pb$_2M^{3+}M'^{4+}$O$_6$ systems ($M'$: magnetic transition metal) for further finding of new magnetic ferroelectric compounds.

![Figure 3. Takata working on the ferroelectric property measurement system.](image3)
Division of Materials Chemistry  
- Chemistry of Polymer Materials -

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Chinese Academy of Sciences, China, 17 November 2004
Prof. MÜLLER, Axel H. E.  
Bayreuth University, Germany, 10 December 2004

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 2004)

Presentations
Structure and Properties of HDPB Formed by LRP (Invited Lecture), Fukuda T, and Rate Retardation in RAFT polymerization, Goto A, and 1 other presentation, 40th World Polymer Congress, France, 4 - 9 July.
2 presentations, 2nd Trilateral Workshop on Organic Chemistry, Kyoto, 4 - 6 September.

Grants
Kinetic Studies on Activation Processes for Organotellurium- and Organostibine-Mediated Living Radical Polymerizations

Organotellurium- and organostibine-mediated LRP (TERP and SBRP, respectively) are new classes of LRP that can provide low-polydispersity polymers in a robust way. The basic concept of LRP is reversible capping of the propagating radical (P\(^+\)) with a capping agent (X) to form a dormant species (P-X), and a prerequisite for achieving low polydispersity is a sufficiently high frequency of activation (decapping of X). In this regard, we determined the activation rate constants for TERP (X = TeMe) and SBRP (X = SbMe) by the gel permeation chromatography (GPC) method (Figure 1) and established their activation mechanisms. The activation for the TERP of styrene mainly occurred by the degenerative chain transfer (DT) between P-X and P\(^+\) with a small contribution of the thermal homolysis of P-X. TERP had been believed to be driven by thermal homolysis and thus conducted at high temperatures, but the kinetic result suggested that, with the addition of conventional radical initiator to supply P\(^+\), TERP can be controlled at lower temperatures with a sufficiently high polymerization rate. This new protocol was confirmed to be effective. The C\(_{n}\) significantly depended on polymers, increasing in the order of methyl methacrylate < styrene < methyl acrylate. For the SBRP of styrene, DT was the only important activation mechanism. The C\(_{n}\) was about twice as large as that for the TERP of styrene, explaining why the SBRP has a better polydispersity controllability than the TERP.

![Figure 1. Schematic representation showing the activation, propagation, and deactivation processes in LRP (top) and the evolution of chain length and chain length distribution as followed by GPC (bottom). The activation rate constant was determined by following the decay of the dormant species concentration at the elution count of 30.5 min. This figure is the cover picture of J. Polym. Sci. Part A: Polym. Chem., issue 19, 42 (2004).](image)

Living Radical Polymerization by Polyhedral Oligomeric Silsesquioxane-Holding Initiators:Precision Synthesis of Tadpole-shaped Organic/Inorganic Hybrid Polymers

Incompletely condensed polyhedral oligomeric silsesquioxane with the highly reactive group of trisodium silicate was used for the synthesis of two initiators for atom transfer radical polymerization, one with a 2-bromoisobutyl group (7Ph-Ts-BIE), and the other with a chlorosulfonyl group (7Ph-Ts-CSPE). These initiators were applied to solution polymerizations of styrene and methyl methacrylate (MMA) in the presence of a copper-complex. In both systems, polymerization proceeded in a living fashion, as indicated by the first-order kinetics of monomer consumption, the evolution of molecular weight in direct proportion to monomer conversion, the good agreement of molecular weight with the theoretical one, and the low polydispersity (Figure 2), thus providing tadpole-shaped polymers with an “inorganic head” of polyhedral oligomeric silsesquioxane (POSS) and an “organic tail” of well-defined polymer. Thermogravimetric and differential scanning calorimetric studies showed that both thermal degradation and glass transition temperatures of the organic/inorganic hybrid polymers with molecular weights up to about 20,000 were enhanced as compared to those of model polymers without the POSS moiety.

![Figure 2. Evolution of number-average molecular weight (M\(_n\)) and polydispersity index (M\(_w\)/M\(_n\)) of POSS-PADMA as a function of monomer conversion for the solution polymerization of MMA (50 wt %) in anisole at 70°C with 7Ph-Ts-CSPE. The full line in Figure 2 represents the theoretical prediction calculated as the molar ratio of polymerized monomer to the initiator.](image)

Tsujii Y, Nanostructure Control by Mixed Polymer Brushes, Grant-in-Aid for Exploratory Research, 1 April 2003 - 31 March 2005.

Goto A, Chain Length Dependence of k\(_t\), Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.


Division of Materials Chemistry
- Chemistry of Polymeric Functionality Materials -

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

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Visitors
Dr SCHAPER, Andreas  Philips University in Marburg, Germany, 25 January - April 18 2004
Dr TRACZ, Adam  Center of Molecular and Macromolecular Studies, Polish Academy of Sciences, Poland, 12 March 2004
Mr WU, Ming-Chien  National Cheng Kung University, Taiwan, 5 July - 30 August 2004
Prof FAN, Zenglu  Xi’an University of Engineering Science and Technology, P.R. China 5 August 2004 - 29 January 2005
Dr KRACOVSKY, Ivan  Charles University, Czech Republic, 30 August 2004 - 30 June 2005
Prof ISMAIL, Hanafi  University Sains Malaysia, Malaysia, 14 - 31 December 2004

Scope of Research

Relationships between molecular arrangements and properties in polymeric functionality materials are investigated through electron microscopic observations and X-ray diffraction measurements elucidating the mechanism of higher-order structural formation. We focus on the studies of the role of crystallites in soft materials such as a natural rubber and a polymer gel. The major research subjects are as follows: (1) Strained-induced crystalization of natural rubber, (2) Ionic conductivity of uniaxially stretched elastomer, (3) Direct observation of molecular chains in the epitaxially grown lamellar crystals of polymers, and (4) Polymer gel consisting of the stereoregular polystyrene.

Research Activities (Year 2004)

Presentations
“High molecular weight branched poly(oxyethlene) as ion conducting elastomers”, Kohjiya S, 5th Symposium of Fundamental Studies for Fabrication of All Solid State Ionics Devices, Tokyo, 28-29 January and other 3 presentations.

Nano-structural Observation of In Situ Silica in Natural Rubber Matrix by Three Dimensional Transmission Electron Microscopy

Three dimensional (3D) nanostructures of particulate silica in natural rubber (NR) were observed for the first time by use of 3D transmission electron microscopy (3D-TEM), which is a combination of TEM with computer tomography, namely electron tomography. The method enabled us to visualize and evaluate structural characteristics in 3D space, such as the size and the volume of in situ silica generated in the NR matrix by the sol-gel reaction of tetraethoxysilane, at nanometer scale resolution.

![Image](image1)

**Figure 1.** Colored volume rendered 3D views of the reconstructed mass density distribution of the silica inclusions for NR-mix-V and NR-in situ-V after removal of zinc compounds. The individual silica particles and aggregates were isolated from the neighbors by coloring. The frame is shown in reconstructed perspective geometry (length and width: 650 nm, thickness: 181 nm). The bar for each direction shows the distance of 100 nm.

Ionic Conductivity of Uniaxially Stretched Poly(oxyethylene)

Elastomers are a group of materials with great deformability upon application of even a small stress. From this point of view, we study the effect of uniaxial stretching of the branched or linear poly(oxyethylene) (PEO) on ionic conductivity. From the relationship between the lithium ion conductivity along the stretching direction and the draw ratio of PEO films, we found the ionic conductivity increased with an increase of draw ratio at various lithium salt concentrations. The *in situ* measurements of wide angle X-ray diffraction using a strong X-ray source from a synchrotron radiation revealed that the degree of orientation of the crystalline chain of PEO was increased continuously with an increase of the stretching ratio.

![Image](image2)

**Figure 2.** Ionic conductivity measurements with uniaxially stretched PEO.


“Past and future of natural rubber”, Kohjiya S, Memorial lecture, 50th Meeting on Polymer Research, Kobe, 15-16 July and other 2 presentations.


**Grants**


Kohjiya S, Feasibility investigation of all solid-state polymer electrolyte film, The funded research from NIC Corporation, 1 January - 30 June 2004.
Division of Materials Chemistry
- Inorganic Photonics Materials -

Prof YOKO, Toshinobu (D Eng)
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TOMOYOSHI, Yoshio (RF)

Visitor
Prof INNOCENZI, Plinio  University of Sassari, Italy, 24 September 2004

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

Research Activities (Year 2004)

Presentations
Na environment in sodium silicate glasses by $^{23}$Na MQMAS NMR spectroscopy and ab initio MO calculation, Tokuda Y, Takahashi M and Yoko T, XX International Congress on Glass, Japan, 16 September - 1 October.

Photochemical reactions responsible for photorefractive index change in germanosilicate glasses, Takahashi M, Tokuda Y, and YOKO T, ibid.

Organic-inorganic low-melting glasses for photonic applications, Takahashi M, Tokuda Y, and Yoko T, ibid.

Relationship between viscoelastic properties and structure of organic-inorganic hybrid glass and supercooled liquid consisting of $R_{6}mSiO_{n-m}$ units, Kakiuchida H, Takahashi M, Masai H, Tokuda Y, and Yoko T, ibid.


Reaction of phosphoric acid and chlorosilane as an acid-base pair for the formation of organic-inorganic hybrid low-melting glasses, Mizuno M, Takahashi M, Tokuda Y, and Yoko T, ibid.

Effect of the organic groups on the formation of siloxane network through sol-gel melting method, Masai H, Takahashi M, Tokuda Y, and Yoko T, ibid. Low-power density laser fabrication of microstructures in low-melting glass doped with rare earth ions as an ion heat, Takahashi M, Sario M, Kakiuchida H, Tokuda Y, and Yoko T, International conference on photoexcited and photoactivated processes, Lecce, Italy, 4 - 10 September.

Low-melting hybrid siloxane glasses containing very small amounts of silanol and alkoxy groups, Masai H, Takahahsi M, Tokuda Y and Yoko T The American Ceramics Society Glass and Optical Materials Division Meeting incorporating the XIV International Symposium on Non-oxide glasses and Novel Optical Glasses, Cape Canaveral, USA, 7 - 12 November.
Laser Micro-fabrication of Organic-inorganic Hybrid Low-melting Glasses Doped with Rare Earth Ions as an Ionic Heater

A new family of low-melting glasses has recently been reported by our group. The organic-inorganic hybrid low-melting glass of SnO-Me₂SiO₂2-P₂O₅ system can be prepared through the non-aqueous acid-base reaction, in which the glass network linkages are produced by Lewis acid-base reaction between H₂PO₄ or H₃PO₄ as Lewis acid and Si(CH₃)₄Cl₂, SnCl₂ or other metal chloride as Lewis base. The obtained glasses showed a high optical transparency and high solubility of organic dyes and optically active ions. Therefore, this glass system is expected to be one of the potential candidate materials for active optical devices. We demonstrated the laser micro-fabrication of the low-melting hybrid glasses doped with neodymium ion (Nd³⁺) by photo-induced refractive index change initiated by a low-power density cw Ar⁺ laser. During this process the irradiated part is locally heated up above their melting temperatures, and then cooled down by turning off the laser beam, resulting in the fictive temperature or local structure of the irradiated region different from that of the non-irradiated part. The photoinduced refractive index change was estimated to be of the order of Δn = -2×10⁻⁵ with a MZ interferometer. Moreover, we have succeeded in fabricating waveguide or phase grating structures inside the hybrid low-melting glass as shown in Fig.1.

![Image](image1.png)  
**Figure 1.** Phase grating structure written inside the low-melting glass by laser heating through nonresonant phonon emission of an excited rare earth ion. Insert shows the diffraction of He-Ne laser light by the phase grating. (The higher order diffractions are also clearly observed.)

Preparation of organic-inorganic hybrid polysiloxane low-melting glasses with high transparency in the uv region, Kuniyoshi M, Takahashi M, Tokuda Y and Yoko T, ibid.

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.


Inhomogeneous Distribution of Na Ion in Mixed Alkali Silicate Glass

We have investigated local structure of Na ion in sodium silicate glasses and mixed alkali silicate glasses by means of ²³Na multiple quantum magic angle spinning (MQMAS) NMR spectroscopy and ab initio molecular orbital (MO) calculation. The ²³Na MQMAS NMR spectra of Na₂O-2SiO₂ have shown an inhomogeneous distribution of local structures around Na as shown in Fig. 2. The MO calculations on the model clusters of sodium silicate glass (Fig. 3) have indicated that there are both the crowded and isolated Na sites in sodium silicate glass. We have also investigated the local structure around Na in mixed alkali silicate glasses, (Na₂O-K₂O)₂SiO₂. ²³Na MQMAS spectra of these glasses have also shown that the addition of K ion makes Na ion occupy more ionic site in mixed alkali silicate glasses. The present study suggests that a cation with a higher ratio of charge to ionic radius tends to aggregate in mixed silicate glasses.

![Image](image2.png)  
**Figure 2.** ²³Na MQMAS spectrum of Na₂O-2SiO₂ glass. MAS dimension and isotropic dimension are presented in ppm relative to an external reference of 1 mol/L NaCl solution. Insert two lines represent chemical shift (QS) and quadrupole interaction shift (QS).

![Image](image3.png)  
**Figure 3.** Optimized clusters modeling (a) isolated Na ion and (b) crowded one. The calculated chemical shifts of model (a) and (b) are -566.2 and -566.6 ppm, respectively. The quadrupole shifts are calculated as 0.5 and 3.3 ppm for model (a) and (b), respectively. All these calculations were performed at the HF/6-31G* level.
Division of Materials Chemistry
- Magnetic Materials -

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

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(D Sc)

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WATANABE, Shinichi (M1)

Visitors
Prof FERRE, J
Laboratoire de Physique des Solides, Universit Paris-Sud, Orsay, France, 13 May 2004

Prof HAASENDONCK, C.
Laboratory of Solid-State Physics and Magnetism, Katholieke Universiteit Leuven, Belgium, 21 May 2004

Prof WUNDERLICH, J.
Hitachi Cambridge Laboratory, UK, 18 November 2004

Scope of Research

The conventional electronics utilizes only the “electric charge” of electrons. On the other hand, the conventional magnetic devices utilize only the “spin” of electrons. A new field of electronics called spintronics, in which both “charge” and “spin” of electrons are utilized in solid-state devices, has been rapidly developing. We are searching for new functional materials which lead to developments of novel spintronic devices by using fabrication techniques such as film growth in units of atom and electron-beam lithography with a resolution of several tenth nano-meters.

Research Activities (Year 2004)

Presentations
Current-driven domain wall motion in magnetic nanowires, Ono T, IFCAM workshop on Nanoscience Nano-technology, 3 - 5 March 2004, Sendai, Japan.


Current-driven domain wall motion in magnetic nanowires, Ono T, 5th International Symposium on Metallic Multilayers, 7 - 11 June 2004, NIST, Boulder, USA.

Electrical spin injection in Ni8Fe15/Al/ Ni8Fe15 double tunnel junctions, Miura K, Ono T, Nasu S, 5th International Symposium on Metallic Multilayers, 7 - 11 June 2004, NIST, Boulder, USA.

NIST, Boulder, USA.

Propagation of a Magnetic Domain Wall in Submicron Magnetic Wires with Asymmetric Notches, Himeno A, Okuno T, Ono T, 5th International Symposium on Metallic Multilayers, 7 - 11 June 2004, NIST, Boulder, USA.

Spin Structure of Cr in Cr/Sn Multilayers with bcc(110) orientation, Jiko N, Mibu K, Takeda M, 5th International Symposium on Metallic Multilayers, 7 - 11 June 2004, NIST, Boulder, USA.

MFM study on current-driven domain wall motion in ferromagnetic nano-wires, Ono T, 7th Oxford-Kobe Materials Seminar, 2 - 4 September 2004, Kobe Institute, Kobe, Japan.


Grants
Ono T, Dynamics of a single domain wall in artificially structured magnetic wires, Grant-in-Aid for Scientific Re-
Current-driven Domain Wall Motion in Magnetic Nanowires

Manipulation of a magnetic state by a spin-polarized current is one of the exciting topics in solid state physics. We succeeded in driving a magnetic domain wall (DW) in magnetic nanowires by flowing an electric current through the wire. Figure 1 shows the real-space observation of this current-driven DW motion by using the magnetic force microscopy (MFM). These are successive MFM images with one pulsed-current applied between each consecutive image. The current density and the pulse duration were 6.7 \times 10^{17} \text{ A/m}^2 and 0.5 \mu s, respectively, and the current direction was from left to right. Here, a DW in the wire is imaged as a dark contrast. The directions of the magnetization in the wire were indicated by the blue and red arrows. This result shows that an electric current can drive the DW and change the magnetic configuration without a magnetic field. We can control the DW position in the wire by tuning the intensity, the duration, and the polarity of the pulsed-current.


Figure 1. Real-space observation of the current-driven domain wall motion by a magnetic force microscopy.

Spin-injection into Non-magnetic Metal

Creation, transport and detection of spins are building blocks of spintronics. The efficient spin injection, accumulation, and transport are central issues to be explored in manipulating the spin degree of freedom of electron. We performed spin injection experiments for Ni_{81}Fe_{19}Au/ Ni_{81}Fe_{19} with double tunnel junctions. Figure 2 shows a scanning electron microscope image of the sample and the geometry of the non-local transport measurements. The sample was fabricated on thermally oxidized Si substrates by electron-beam lithography for patterning, oblique deposition, and lift-off method. The sample has two Au/Al_{2}O_{3}/ Ni_{81}Fe_{19} tunnel junctions at the overlap of the Al wire and the Ni_{81}Fe_{19} wires. A current I enters from the left Ni_{81}Fe_{19} electrode and is extracted at the left end of the Al wire. Spin polarized electrons injected from Ni_{81}Fe_{19} into Al create nonequilibrium spin accumulation in Al. This spin accumulation is detected as voltage V measured between the right Ni_{81}Fe_{19} electrode and the right end of the Al wire. Figure 3 shows the spin-signal V/I at 10 K as a function of a magnetic field. The measurements were performed by DC four terminal method using a current of I = 5 \mu A. The configuration of magnetizations of Ni_{81}Fe_{19} electrodes are schematically indicated by arrows in the figure. The sign of the spin-signal V/I reverses when the relative magnetization configuration between two Ni_{81}Fe_{19} electrodes changes from parallel to anti-parallel, indicating the existence of the difference in electrochemical potentials between the spin-up and spin-down electrons injected from Ni_{81}Fe_{19} into the Al wire.

Figure 2. SEM image of the spin injection and detection device, with the geometry of the non-local measurement.

Figure 3. Spin-signal V/I for Ni_{81}Fe_{19}Au/Ni_{81}Fe_{19} as a function of magnetic field at 10 K.

search (C) (2), 1 April 2003 - 31 March 2005.
Ono T, Nanospintronics Design and Realization, MEXT Special Coordination Funds for Promoting Science and Technology, 1 September 2002 - 31 March 2005.

Award
Division of Biochemistry  
- Biofunctional Design-Chemistry -  
http://www.ecl.kyoto-u.ac.jp/sugiura/index.html

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Visitors
Prof VIVES, Eric  
University of Montpellier II, France, 16 February 2004
Dr MIHALA, Nikolett  
Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary, 27 July - 31 August 2004
Prof DIBO, Gabor  
Institute of Chemistry, Eotvos L, University, Hungary, 22 October 2004
Prof HUDECZ, Ferenc  
Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary, 23 October - 4 November 2004
Prof MICHEL, L. J. Sarah  
Maryland University, USA, 16 November 2004

Scope of Research
As an interface of chemistry and biology, this division investigates the molecular mechanism of specific interaction between biologically active molecules and macromolecular receptors. We also aim at the design of novel functional molecules. Current research subjects are as follows: (1) Elucidation of the DNA recognition mode of C2H2-type zinc finger proteins and design of artificial DNA binding peptides. Studies on the structure and function of a zinc finger motif by coordination of a metal. (2) Design and synthesis of artificial functional peptides and development of novel intracellular delivery systems aiming at elucidation and control of cellular functions.

Research Activities (Year 2004)
Presentations
Artificial Zinc Finger Proteins: Designs and Functions, Sugiura Y, Special Seminar of Risbon University, Risbon, Prortogal, 15 March.
Delivery of macromolecules into cells using non-viral vectors, Arginine-rich peptides: aspects of membrane translocation, Futaki S, Molecular design of drug delivery and development symposium series, Toronto, Canada, 9 - 10 July.
Creation and Function of Zinc Finger Proteins, Sugiura Y, 31st Organi Reaction Meeting, Kyoto, 31 July.

Grants
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.
Sugiura Y, Creation and DNA binding of the longest
Metal-mediated Modulation of Peptide Structure and Recognition

Helical peptide segments that alternate their conformation in accordance with external stimuli are attractive building blocks for the development of novel peptide devices and materials. Substantial efforts have been focused on stabilizing the helical structure by metal chelation and ion pair formation. However, approaches to destabilize peptide structures may be promising for the helices having a strong tendency of helix formation. We have prepared helical peptides equipping a pair of the iminodiacetic acid derivatives of lysine (Ida), and showed the importance of the topologies of the Ida residues for helix stabilization and destabilization. For the preparation of Ida-containing peptides, we developed a novel approach using the direct conversion of Lys to Ida on the Fmoc-solid phase resin. When the Ida residues were placed at 1 and 1+2 positions in a 17-residue helical peptide, the addition of Fe(III) resulted in a significant decrease in the helical content whereas Fe(II) had no influence on the helix stability. The possibility of redox control of the helical structure was then exemplified by the reduction of Fe(III) to Fe(II) using Na2S2O4 followed by the subsequent reoxidation. Mutual recognition between the transcription factor Jun-derived leucine-zipper peptide segment and the Fos-derived one containing Ida residues was also modulated in the presence of Fe(III). The concept of structural switching by helix destabilization would open new avenues for the design of novel peptidobased functional molecules and devices.

Exchange of Histidine Spacing between Sp1 and GLI Zinc Fingers: Distinct Effect of Histidine Spacing-Linker Region on DNA Binding

A C3H2-type zinc finger has a tandemly-repeated structure, which consists of independent modules with the consensus sequence, ((Tyr, Phe)-X-Cys-X2,4-Cys-X2-Phe-X3-Leu-X2-His-X2,3-His-X2), Each domain forms a compact bba structure held together tetrahedrally by coordination of a zinc ion with two invariant cysteines and histidines. Typical C3H2-type zinc fingers recognize the three-base-pair subsite mainly on one strand using key amino acid residues of the a-helix. Based on these features, new zinc fingers with various sequence specificities have been designed by mutating amino acid residues in the a-helix by rational structural design and by a phage-display-based method. In the DNA recognition mode of C3H2-type zinc fingers, the finger-finger connection region, consisting of the histidine spacing and linker, would be important for determining the orientation of the zinc finger domains. The histidine spacing is conserved from HX3H to HX5H and has various conformations in accordance with the number of amino acid residues. On the basis of the previous structural analyses, an HX3H-type spacing forms a 310-helix, whereas HX4H-type and HX5H-type spacings form helical structures. The local conformational alteration of the histidine spacing might result in changing the DNA binding of zinc finger proteins. In order to clarify the influence of spacing between two ligand histidines in the DNA binding, we exchanged the histidine spacing between Sp1 and GLI zinc fingers, which have an HX3H-TGEKK linker (typical) and an HX4H-SNEKP linker (atypical), respectively (Figure 1). A significant decrease in the DNA binding affinity and specificity is found in Sp1-type peptides, whereas GLI-type peptides show a mild reduction. To evaluate the effect of the linker characteristics, we further designed Sp1-type mutants with an SNEKP linker. As a result, the significant effect of the histidine spacing in Sp1-type peptides was reduced. These results demonstrate that (1) the histidine spacing significantly affects the DNA binding of zinc finger proteins and (2) the histidine spacing and the following linker regions are one effective target for regulating the DNA recognition mode of zinc finger proteins.

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Division of Biochemistry
- Chemistry of Molecular Biocatalysts -

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Anhui Agricultural University, China, 16 May 2004
Dr. FLEISCHMANN, Hans-Peter
Technical University of Braunschweig, Germany, 12 October 2004
Dr. HAZARIKA, M., Mr. PRAKASH, Sudhir
Tea Research Association, India, 16 November 2004

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

Research Activities (Year 2004)

Presentations
Diglycosidases specifically hydrolyzing disaccharide glycosides in plants, Mizutani M, Ahn Y-O, Saino H, Sakata K, 44th Symposium on the Chemistry of Natural Products (Hiroshima), 6 - 8 October.
Tracer Analysis of the Oxidation Steps in Biosynthesis of Coumarins in Sweet Potato using $^{18}$O$_2$

Sweet potato (Ipomoea batatas L.) accumulates umbelliferone and scopoletin after wounding or pathogen infection. The biosynthetic pathway of the coumarins remains unclear and is supposed to be biosynthesized via a phenylpropanoid pathway. To explain the oxidation of the 2'-position during coumarin formation, feeding experiments to sweet potato were performed with stable isotope oxygen ($^{18}$O$_2$). The sweet potato discs treated with chitosan (1 mg/ml) as an inducer were exposed to the artificial air consisted of N$_2$, $^{18}$O$_2$ and CO$_2$ for 24 hr, and the accumulated umbelliferone was analyzed by ESI-LC/MS$^3$. The pseudomolecular ions [M+H]$^+$ of umbelliferone (M.W. 162) were detected at m/z 163 (100%), 165 (45), 167 (27). The pseudomolecular ion m/z 163 gave the fragments m/z 107, 119, 135 on the MS$^3$ spectrum after N$_2$ collision. Under the same conditions, the pseudomolecular ion m/z 165 and 167 also gave a set of the fragments m/z 109, 119, 121, 137 and 109, 121, 139, respectively. In the control without $^{18}$O$_2$, intensities of the ions m/z 165 and 167 were 80% and 74% weaker than those of the discs treated with $^{18}$O$_2$, respectively. The control discs incubated in H$_2$O similarly gave weaker intensities of these ions, indicating $^{18}$O in the ions m/z 165 and 167 is not from H$_2$O. These data indicate that $^{18}$O$_2$ is taken up into not only 4'-position but also 2'-position of the trans-cinnamate during the umbelliferone formation. These facts imply the existence of the enzyme(s) that catalyzes 2'-hydroxylation on the benzene ring of p-coumarate using O$_2$ (Figure 1).

Directed Evolution of Lipase for Improved Amidase Activity

Lipases are the serine hydrolases that have extraordinarily broad substrate specificity and high enantioselectivity for the hydrolysis of structurally diverse esters. Despite the similarities of lipases to serine proteases in the active site structure and the reaction mechanism, lipases do not hydrolyze amides, whereas serine proteases hydrolyze amides as well as esters. We have engineered a lipase from Pseudomonas aeruginosa for improved amidase activity by a directed molecular evolutional technique. A gene encoding the lipase was randomized by error-prone PCR, and the mutants were screened for improved amidase activity for oleyl 2-naphthylamide. From a total of 20,000 mutants, six clones were found to have increased relative amidase activity (Figure 2). DNA sequencing of the mutant genes identified three mutations, F207S, A213D and F265L, responsible for improved amidase activity. The combination of these mutations indicated that a double mutant F207S/A213D gave the highest molecular amidase activity of 1.1 min$^{-1}$, a 2-fold increase in amidase activity as compared to the wild-type lipase. A structural model indicated that the mutations occurred at the sites near the surface and remote from the active site, but were close to the calcium binding site (Figure 3). This study is a first step towards the preparation of a general acyl-transfer catalyst for the biotransformation of amides.

Figure 1. Tracer analysis of the oxidation steps in biosynthesis of coumarins in sweet potato using $^{18}$O$_2$

Figure 2. Amide- and ester-hydrolyzing activities (vs, amide and vs, ester) of mutant lipases

Figure 3. Structural model of lipase

Grants

Award
Saito S, The ICR Award for Young Scientist, ICR, 3 December 2003.
Division of Biochemistry
- Molecular Biology -

Prof OKA, Atsuhiro (D Sc)
Assoc Prof SUGISAKI, Hiroyuki (D Sc)
Assoc Prof AYOYAMA, Takashi (D Sc)
Assist Prof TSUGE, Tomohiko (D Sc)
Assist Prof SAKAI, Hiroe (D Sc)

Res Associate OHASHI, Yohhei (D Sc)
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TABATA, Satoshi (D Sc)
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Students
TANIGUCHI, Masatoshi (D3)
IMAI, Kumiko (D2)
YAMAMOTO, Yukimi (D1)

Visitors
Prof BANKAITIS, V.A.
University of North Carolina, Chapel Hill, USA, 26 April 2004
Prof QU, L.-J.
Peking University, Beijing, China, 6 - 7 August 2004

Scope of Research

This laboratory aims at clarifying the framework of regulatory network between genetic programs and environmental stress responses through the study on structure-function relationships of genetic materials and cellular proteins in higher plants and pathogens. The major subjects are mechanisms involved in intracellular signal transduction and regulation of gene expression responsive to environmental stimuli, differentiation and development of plant organs, and plant-microbe interaction. As of December 2004, study is being concentrated on the two-component response regulators involved in cytokinin signaling, HD-Zip proteins required for phospholipid signaling, COP9 signalosome modulating protein degradation, and cyclines and CDKs controlling cell cycle.

Research Activities (Year 2004)

Presentations
Sequence structure recognized by the Arabidopsis response regulator ARR1, Taniguchi, M; Aoyama, T; Oka, A; Expression analysis of the AtPLD2 gene in Arabidopsis thaliana, Yamamoto, Y; Ohashi, Y; Oka, A; Aoyama, T, 2004 Ann Meeting of Jpn Soc Plant Physiol, 27 - 29 March (Hachioji).
Targets of ARR1, Aoyama, T, International Workshop on Cytokinin Metabolism, Signaling and Function, 10 July (Berlin, Germany).
Interaction between CSN1 (COP9 Signalosome subunit 1) and components of transcription/RNA processing complexes SAP130, DDX15/Prp43/mDEAH9, and CFLm68, Menon, S; Tsuge T et al., 2004 FASEB Summer Research Conference at Vermont Academy, 14 - 19 August (Saxtons River, VT USA).
Contribution of phospholipase D to morphogenesis of plant epidermal cells, Oka, A; Ohashi, Y; Aoyama, T, 2004 Ann Meeting & Symposia of Genetics Soc Jpn, 27 - 29 September (Suta).
Role of phospholipase D in root-hair cell morphogenesis, Ohashi, Y et al., European Plant Science Organization Conference: Interactions in Plant Biology: cells, plants and communities, 10 - 14 October (Ischi, Italy).
Hunting target genes of Arabidopsis transcription factors, Aoyama, T, Workshop at University of Rome La Sapienza, 18 October (Rome, Italy).
The Challenge on Revealing the Novel Regulation of COP9 Signalosome; a Master Regulator of Plant Signal Transduction

Survival of a life-form largely depends on how it perceives the environmental information and what it does in response. Higher plants, unlike many animals, spend most of their lives immobilized at a single location. Consequently, plants have acquired a high degree of plasticity during evolution, giving unique regulation of morphogenesis in response to environmental signals. Among such signals, evidently, light is the key signal for plant development and survival. A genetic screen with *Arabidopsis thaliana* has revealed a set of cop/det/fas mutants possessing light grown seedling phenotype in the dark. The ten responsible COP/DET/PUS genes are negative regulators of photomorphogenesis in darkness. Among these genes, six code for the subunit proteins of a large nuclear protein complex called the COP9 Signalosome (CSN).

CSN is not specific to plants but highly conserved in a broad range of animals where light signal has less influence on morphogenesis. Interestingly, each of the eight subunits of the CSN has structural conservation with one of the eight subunits in the Lid-subcomplex of the 26S Proteasome, the machinery for ubiquitin-mediated protein degradation. These two complexes are paralogous to each other, suggesting an evolutionary relationship (left figure). Individual subunits of the CSN has been linked to various signal pathways leading to gene expression regulation and cell cycle control.

We previously found that CSN interacts with the E3 ubiquitin ligases and regulates the ubiquitin-proteasome degradation pathway by releasing the covalent bond between a small ubiquitin-like protein (plant Rubi1 or animal NEDD8) and the Cullin subunit of the E3 ligase [1]. This regulatory system of phosphorilase involved in cytokinin signaling, Grant-in-Aid for Scientific Research (B), 1 April 2004 - 31 March 2007.

Aoyama T, Molecular mechanism of adaptive responses controlled by *Arabidopsis* His-Asp phosphorilase signal transduction, Grant-in-Aid for Scientific Research on Priority Areas (B), 1 April 2000 - 31 March 2005; Roles of phospholipid signaling in root-hair formation, Grant-in-Aid for Scientific Research (B), 1 April 2004 - 31 March 2007.

Role of phospholipase D in plant cell morphogenesis, Yamamoto Y, Ohashi Y, Oka A, Aoyama T; *Arabidopsis* AtCycA2; 3 is a key regulator of termination system of endoreduplication, Imai K et al., 2004 Ann Meeting of Mol Biol Soc Jpn, 8 - 11 December (Kobe).

Grants

Oka A, Molecular basis of cytokinin signaling in plant cells, Grant-in-Aid for Scientific Research on Priority Areas (A), 1 April 2003 - 31 March 2005; Two-component
Scope of Research

This laboratory was founded in 1994 with the aim of linking biochemical 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-ribose)lation in protection of genome from apoptosis-inducing stresses, the physiological and pathological functions of brain-specific septin, and the molecular etiology of neurodegenerative disorders including Alzheimer’s disease and Parkinson’s disease.

Research Activities (Year 2004)

Presentations


A Pathological Role of CYP2D6 Gene as a Risk Factor for Parkinson’s Disease, Tanaka S, Takehashi M, Matoh, N, and Ueda K, 11th Annual Meeting of the Japanese Society for Gene Diagnosis and Therapy, Tokyo, 17 - 18 September.


A Role of Poly(ADP-ribose) Polymerase-1 in Ischemic Neuronal Cell Death

Poly(ADP-ribose) polymerase-1 (PARP-1), a nuclear enzyme also known as poly(ADP-ribose) synthetase, is activated by DNA strand breaks and forms (ADP-ribose)_{n} chains from NAD^{+}. Ischemic brain injury activates PARP-1 and results in neuronal cell death. A 2-h oxygen-glucose deprivation (OGD) followed by reoxygenation induced apoptosis of rat cortical neurons in culture. Overexpression of a mitochondrial antiapoptotic protein, Bcl-2, efficiently protected the cells from OGD-Reox-induced apoptosis, implying mitochondrial impairment in this process. To support this, the OGD was found to bring about mitochondrial permeability transition (MPT), or membrane depolarization, and a release of proapoptotic proteins from mitochondria. Of the proteins released, cytochrome c was distributed in the cytoplasm and activated a caspase cascade, leading to PARP-1 cleavage in the nucleus. In contrast, apoptosis-inducing factor (AIF) and endonuclease G translocated themselves into the nucleus. Both the MPT and protein translocation were efficiently attenuated by PARP-1-specific inhibitors, 1,5-dihydroxyisoquinoline and benzamidine. Knocking down the PARP-1 gene expression with small interfering RNA also protected the cells from apoptotic changes in mitochondria as well as the nucleus. These results indicated a mechanism of ischemia and reperfusion injury in which PARP-1 plays a principal role in inducing mitochondrial impairment, which ultimately leads to apoptosis of neurons.

Suppression of Chemical-Induced Cell Death by Poly(ADP-ribose) Polymerase-1 Inhibitors

The purpose of the present study was to determine whether 6(5H)-phenanthridinone, a potent inhibitor of PARP-1, could attenuate the hepatotoxicity of carbon tetrachloride (CCl_{4}). Male ICR mice treated via the intraperitoneal route with CCl_{4} exhibited severe necrotic centrilobular lesions and significantly elevated serum transaminases. In contrast, the histopathology and serum biochemistry of animals treated concomitantly with CCl_{4} and 6(5H)-phenanthridinone were not significantly different versus controls. In conclusion, the results of this study demonstrate that the hepatotoxicity of CCl_{4} can be blocked independently of its metabolism and suggest the predominant role of PARP-1 overactivation in chemical-induced toxicity.

Expression, Distribution, and Complex-Formation of Septin 3 Isoforms in Human Brain

Septin 3 is a member of a family of highly conserved 40-60 kDa GTPase-domain proteins called septins. Human septin 3 was originally cloned as a gene up-regulated upon neuronal differentiation of a human teratocarcinoma cell line NT2. More recently, we found a genetic association of septin 3 polymorphisms with Alzheimer’s disease. Alternative splicing of the septin 3 gene transcript produces two isoforms, A and B, in the human brain, though their regional expression and physiological function remain to be determined. In the present study, we analyzed the expression patterns of human septin 3 isoforms in normal human brain and a human neuroblastoma cell line, SH-SY5Y, after retinoic acid-induced differentiation. The expression and distribution of septin 3 isoforms A and B were similar and resembled those of another septin, CDCrel-1. Septin 3A and 3B were expressed in normal human brain in a region-specific manner with the highest level in the temporal cortex and hippocampus and the lowest level in the brainstem regions. Prominent immunoreactivity was observed diffusely in the neocortices in association with neuropils and punctate structures suggestive of synaptic junctions. Immunoprecipitation studies revealed that septin 3A, 3B, and CDCrel-1 form a complex in the frontal cortex of human brain. These findings suggest that septin 3A and 3B, along with CDCrel-1, play some important role(s) in synaptogenesis and neuronal development.
Scope of Research

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

Research Activities (Year 2004)

Presentations
Solid-State NMR Investigations of Alq3 in Different Polymorphs, Kaji H, International Discussion Meeting on Tris(8-hydroxyquinoline)aluminum(III), 22 September (Invited).
Precise Solid-State NMR Analysis of Polymers and Metal Complex Light-Emitting Materials and the Control of their Optical Properties, Kaji H, 45th Symposium on Coordination Chemistry, Jpn., 23 September (Invited).
Solid-State NMR Investigations of facial and meridional Alq3 in Different Polymorphs, Kaji H, 21COE Workshop on OSE & OEL (Mark Thompson Symposium), 30 October (Invited).


Grants
Horii F, Precise Solid-State NMR Analyses of Non-crystalline Organized Structure and Dynamics of Polymer Functional Materials, Grant-in-Aid for Scientific Research
A Combined Experimental and Theoretical Study of the Conformation of TPD Using Solid-State $^{15}$N NMR and DFT Calculations

The conformation of $N,N'$-diphenyl-$N,N'$-di(4-tolyl)benzidine (TPD) (Figure 1), which is widely used as a hole-transport material in organic electroluminescent (OEL) devices, has been studied by solid-state $^{15}$N NMR and density functional theory (DFT) calculations [1]. Solid-state NMR is a suitable tool for the analysis of the organic materials in OEL devices, since the materials are normally in the amorphous state and the detailed structures are hard to access by diffraction methods. Figure 1 shows the DFT-calculated $^{15}$N NMR chemical shift anisotropy (CSA) spans, $\alpha_{m}$ - $\sigma_{m}$, of amorphous TPD plotted as a function of the torsion angles, $\alpha$ and $\beta$. The CSA spans significantly vary depending on the conformation and can be used for the determination of torsion angles. The experimental CSA span of $^{15}$N-labeled amorphous TPD was 15 ppm. This corresponds to the narrowest CSA span among the DFT-calculated values in Figure 1. The DFT-optimized structure with torsion angles $\alpha$ of 40-41° and $\beta$ of 41-43° gives the narrowest CSA span, indicating that the torsion angles determined by the experimental CSA span agree well with those obtained from the DFT-optimized structure. This confirms that the DFT-optimized TPD single molecule reflects the structure in the condensed amorphous state: the nitrogen atom and the three carbons directly bonded to the nitrogen are in the same plane, and three rings attached to the nitrogen adopt a propeller-shape conformation. Forty stable conformers are considered to exist in the amorphous state. Torsion angles change the shape of molecules and the state of the electron clouds around the nitrogens, and therefore significantly affect the intermolecular electron coupling. It suggests that the torsion angle is a crucial factor for the carrier transport properties.

Figure 1. DFT-calculated $^{15}$N $\alpha_{m}$ - $\sigma_{m}$ values of amorphous TPD as a function of torsion angles $\alpha$ and $\beta$.

Phase Behavior of Aqueous Mixture of Cellulose Microfibrils and Imogolite Nanotubes and Preparation of Their Nanocomposites

Development of functional green polymer materials is a subject of great importance. Phase behavior of the mixture of tunicate cellulose microfibrils and imogolite nanotubes in the aqueous solution of acetic acid (pH=3) has been studied to fabricate cellulose-based nanocomposites. Tunicate cellulose microfibrils prepared by sulfuric acid treatment are rodlike. They are 1-3 µm long and 15-30 nm wide. Purified imogolite nanotubes with an outer diameter of 2.5 nm are estimated at 0.3 µm in length. Both cellulose microfibrils and imogolite nanotubes form their own lyotropic mesophases in the aqueous solution of acetic acid. The imogolite solution separates into the isotropic and liquid crystalline phases above the concentration of 0.8% (A point) in the aqueous solution of acetic acid. In contrast, the microfibril suspension becomes turbid without phase separation at 0.3%, and forms only the liquid crystalline phase above 1.5%. Each mixed suspension of microfibrils/imogolite nanotubes with different weight ratios below 1/1 shows the two phases after one day and the volume of the liquid crystalline phase increases with increasing concentration (Figure 2). Characterization of nanocomposite films prepared from respective liquid crystalline phases of microfibrils/imogolite nanotubes with different weight ratios is in progress.

Figure 2. Phase behavior of microfibrils/imogolite nanotubes (1/1) dispersed in the aqueous solution of acetic acid as a function of the total concentration. (a) Immediately after preparation. (b) After 2 months. The turbid phase is the liquid crystalline phase. The concentration of the A point is 0.4%.

(B)(2), 1 April 2004 - 31 April 2006.

Hori F. Hybridization Utilizing Hierarchical Structure of Microbial Cellulose by a Newly Developed Microbiol-system, Grant-in-Aid for Scientific Research, 1 April 2004 - 31 April 2006.


Scope of Research

Research activities are concerned with geochemistry, oceanography, limnology and analytical chemistry, which are important basic sciences in order to realize the sustainable society. Major research subjects are as follows: (i) Biogeochemistry of trace elements in the hydrosphere. (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 2004)

Presentations


Molecular design of solvent extraction reagents highly selective for lanthanide metal ions, Umetani S, International Conference on Rare Earths in Nara, Japan (Rare Earths '04 in Nara), 12 November 2004.


Grants


Okamura K, Development of time-series measurement system of sulfur related matter in seawater, Grant-in-Aid for Young Scientists B, 1 April 2003 - 31 March 2006.
Distributions of Trace Metals in the Sulu Sea (Philippines) and its Adjacent Basins

Distributions of trace metals in seawater can keenly reflect physical, chemical and biological processes occurring in the ocean. The Sulu Sea (the Philippines) is a deep semi-enclosed basin surrounded by shallow sills (<420 m) and lands, and shows temperature of deep water being ~10°C which is higher than that of open ocean. Therefore, the Sulu Sea is quite different from the open ocean and expected to show unique profiles of trace metals. However, few studies have been made for distributions of trace metals in the Sulu Sea. We observed vertical profiles of dissolved and acid dissolvable Fe, Co, Ni, Cu, Zn, Cd concentrations in the Sulu Sea (Stn. 10, 8°30’N 121°48’E, Dec. 2002) and its adjacent seas, such as the South China Sea (Stn. 16, 13°30’N 119°30’E, Dec. 2002), and western part of the Northwest Pacific (BO7, 22°00’N 151°00’E, July 2000) (Fig. 1).

Figure 2 shows vertical profiles of dissolved trace metals. Although profiles of dissolved Ni, Zn and Cd in the Northwest Pacific were nutrient like, concentrations of these metals in the Sulu Sea were more uniform below the subsurface. The average concentrations of dissolved Ni, Cu, Zn, Cd in 1000-4000 m in the Sulu Sea were 6.1, 1.5, 3.7, 0.4 nM and were found to be significantly lower than those obtained from the Northwest Pacific (9.5, 3.2, 10.0, 0.9 nM) and the South China Sea (9.0, 2.7, 9.2, 0.8 nM). The difference is also the case for major nutrients and rare earth elements. Because the North Pacific is near the terminal of deep-water circulation in the World Ocean, deep waters of the Northwest Pacific and its adjacent South China Sea are abundant in regenerated nutrients and trace metals mentioned above. Unlike these basins, deep waters of the Sulu Sea would be hardly influenced by nutrient-rich deep waters because of shallow sills, and existing water masses in the deep layer would originate in shallower layer with lower trace metal concentrations. These results suggest that the Sulu Sea is a unique basin compared to the open ocean not only for temperature and major nutrients, but also trace metals.

Figure 2. Vertical profiles of dissolved Fe, Co, Ni, Cu, Zn and Cd in the Sulu Sea (white circle), the South China Sea (blue circle) and Northwest Pacific (red circle).

Distributions of Dissolved and Acid Dissolvable Bioactive Trace Metals in the Australian Sector of the Antarctic Ocean (2001 - 2002)

Dissolved and acid dissolvable Fe, Co, Ni, Cu, Zn, Cd and Pb were measured in the Australian sector of the Antarctic Ocean (47-66°S, 140°E) from November 2001 to March 2002.

In upper waters (shallower than 200 m), for Co, Ni, Cu, Zn, and Cd, the concentrations of acid dissolvable species mostly agreed with those of dissolved species within an experimental error, but for Fe and Pb, the concentrations of acid dissolvable were significantly higher than those of dissolved species. Profiles of dissolved and acid dissolvable Fe showed a same tendency of variation to depth and reached maximum concentrations at same depths (Fig.3).

Profiles of dissolved concentrations of all the trace metals showed an inter-latitude variation. Influences of Antarctic Divergence, Antarctic Bottom Water and Antarctic Intermediate Water on the concentrations were observed. Concentrations of dissolved Ni, Cu and Cd showed correlations to those of phosphate at all stations.

Among November 2001, February 2002, and March 2002, dissolved concentrations of trace metals in upper waters at 64°S and 61°S were compared to look a seasonal variation. The concentrations of Co, Ni, Cu, Zn and Cd did not show significant change during the observation.

Figure 3. The distributions of dissolved and acid dissolvable Ni and Fe in upper water at 61°S (triangle: dissolved, circle: acid dissolvable).
Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR under extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Static and dynamic NMR of endocrine disruptors, anesthetics, peptides, and proteins in lipid bilayer membranes are also investigated.

Research Activities (Year 2004)

Presentations
A Challenge to Chemical Evolution Using Hot Water, Nakahara M, Workshop on Chemistry of Biological Processes Created by Water and Biomolecules, 9 January.


Grants
Nakahara M, Development of Multinuclear, High-Temperature, and Diffusion-Measurable NMR Probe and Molecular Analysis of Dynamics of Supercritical Aqueous Solutions, Grant-in-Aid for Scientific Research (A) (2), 1
NMR Spectroscopic Evidence for an Intermediate of Formic Acid in the Water-Gas-Shift Reaction

The water-gas-shift (WGS) reaction ($\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$) is investigated in connection to formic acid. Using NMR spectroscopy, the reversible decomposition pathways of formic acid to both sides of the WGS reaction are studied in hot water at 240-260°C. This reversibility strongly suggests that formic acid exists as an intermediate in the WGS reaction, and it is indeed demonstrated that carbon monoxide is treated in hot water to produce formic acid. The present result enables us to generate and store hydrogen in the liquid form of formic acid and to transform formic acid to hydrogen in water by tuning the thermodynamic conditions.

Figure 1. The time dependence of the product yields in the noncatalytic water-gas-shift reaction at 250°C.

Lipid Membrane Dynamics and Drug Transport by High-Field-Gradient, High-Resolution NMR

Diffusion rates of lipids and a trapped endocrine disruptor, bisphenol A (BPA), are determined in fluid lipid membranes. We have specially designed a high-power field gradient probe for a 600 MHz NMR apparatus. The probe can exert a field gradient up to 1350 G/cm, which is sufficient to monitor dynamic events in highly viscous cell membrane. The motion of BPA is not rapid in membrane. The mobility is almost equal to the membrane lipid diffusion. It is in sharp contrast to the motion of benzene and toluene in membrane, which diffuse faster than the lipid matrices (Figure 2). The slowdown of BPA and lipid motions is leveled off in 100- and 400-nm vesicles, although the hydrodynamic continuum model gives the molecular motion slowed inversely to the lipid particle size. Instead, the limited motion is related to the intra-membrane fluidity. Diffusion rates of alkylbenzenes and alkylphenols, anesthetics, and channel peptides are also successfully determined in membranes.


Figure 2. Mobility of drugs in membrane. In the upper graph are the self-diffusion rates of drugs in water (white) and in 100-nm vesicles (red) at 30°C, together with the mobility of membrane lipid head group (light yellow) and the chain core (yellow). Location of the drug in membrane is shown schematically in the bottom by the space filling model with H, blue; C, grey, and O, red.

April 2003 - 31 March 2006.
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.

Award
Nakahara M, Prize of The Japan Society of High Pressure Science and Technology, 2004, NMR Studies on Water and Aqueous Solution under High Pressure and Supercritical Conditions, 10 October.
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 2004)

Presentations


Grants


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

Esaki N, Isolation of novel cold-adapted microorganisms and exploitation of useful gene resources, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2005.

Yoshimura T, Physiological role of D-amino acids in
Phosphoproteome Analysis of a Psychrotrophic Bacterium, *Shewanella* sp. Ac10, to Elucidate Its Cold-adaptation Mechanism

We tried to elucidate the cold-adaptation mechanism of a psychrotrophic bacterium, *Shewanella* sp. Ac10, isolated from Antarctic seawater by phosphoproteome analysis. Membrane proteins were extracted from the cells cultivated at 4°C and 18°C and separated by two-dimensional gel electrophoresis (2-DE). Phosphorylated proteins were detected by staining the 2-DE gels with Pro-Q Diamond and identified by peptide mass fingerprinting. Six and eight membrane proteins were found to be phosphorylated in the cells cultivated at 18°C and 4°C, respectively. One of the proteins phosphorylated at 4°C was identified as a homolog of TolC, which functions as an exit duct in *Escherichia coli*. Although the amount of the TolC homolog was not significantly affected by the cultivation temperature, it was more remarkably phosphorylated at 4°C than at 18°C. We also found two phosphorylated proteins specifically produced at 4°C. These phosphorylated proteins probably play a role in the adaptation of this bacterium to a cold environment.

![Figure 1. Membrane transport systems of *Shewanella* sp. Ac10 grown at 4°C.](image)

Enzymatic Synthesis of N-methyl-L-phenylalanine by a Novel Enzyme, N-methyl-L-amino Acid Dehydrogenase

We found N-methyl-L-amino acid dehydrogenase activity in various bacterial strains, such as *Pseudomonas putida* and *Bacillus alvei*, and cloned the enzyme gene from *P. putida* ATCC12633 to *E. coli*. The enzyme purified to homogeneity from the recombinant *E. coli* catalyzed the NADPH-dependent formation of N-alkyl-L-amino acids from the corresponding α-keto acids (e.g., pyruvate, phenylpyruvate, and hydroxypropyruvate) and alkylamines (e.g., methylamine, ethylamine, and propylamine). An enzymatic system for the synthesis of N-methyl-L-phenylalanine from phenylpyruvic acid and methylamine with N-methyl-L-amino acid dehydrogenase using NADPH and glucose dehydrogenase from *Bacillus subtilis* as a cofactor-recycling system is developed. Analysis of the product of the laboratory preparative scale process revealed N-methyl-L-phenylalanine in 98% yield and over 99% e.e. N-Methyl-L-phenylalanine can be used as chiral building blocks for the synthesis of several products with pharmacological activity.

![Figure 2. The enzyme-catalyzed production of N-methyl-L-amino acid in combination with cofactor-recycling catalyzed by glucose dehydrogenase.](image)

eukaryote, Grant-in-Aid for Scientific Research (C), 1 April 2002 - 31 March 2004.

Kurihara T, Development of a low-temperature protein-production system regulating the formation of inclusion body, Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2006.

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

Mihara H, Mechanisms of incorporation of sulfur and selenium into the anticodon wobble bases of tRNAs, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2006.

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


**Award**

Division of Multidisciplinary Chemistry  
- Polymer Materials Science -

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

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Scope of Research

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

Research Activities (Year 2004)

Presentations


Structure Formation of Polyelectrolyte Solutions by Coulombic Interactions, Nishida K, Kanaya T, Kaji K, 2004 Spring Meeting, the Physical Society of Japan, Fukuoka, 28 March (invited).


Neutron-Spin Echo Studies on Three Types of Poly(vinyl alcohol) Gels, Takahashi N, Kanaya T, Nishida K, Kaji K, UK-JPN Polymer Workshop, Kyoto, 1 April.

Crystallization of Isotactic Polypropylene under Shear Flow, Ogino Y, Matsuba G, Nishida K, Kanaya T, OUMS’04, Osaka, 12 July.


Grants
Kanaya T, Nishida K, Polymer Crystallization under
Nanoscale Dynamics of Polymer Gels

Neutron spin-echo (NSE) technique is a unique tool to study dynamics in nanometer scale. We have investigated dynamic and static fluctuations in three types of poly(vinyl alcohol) (PVA) gels to elucidate the heterogeneity in nanometer scale using NSE spectrometer in JRR-3M reactor in Tokai (Fig. 1). The first one was a PVA gel in a mixture of deuterated dimethyl sulfoxide (DMSO-d6) and D2O with volume fraction of DMSO-d6 being 0.6. On the basis of NSE results, small-angle neutron scattering (SANS) intensity was divided into static and dynamic fluctuations to find that the static fluctuations were dominant in the present Q range (Fig. 2). The second one was PVA in aqueous borax solution. The intermediate scattering functions of the gel as well as the sol were well described by Zimm mode and gel mode in Q regions above and below a critical value Qc, corresponding to the correlation length of the network. The last one was the chemically cross-linked PVA gel. The intermediate scattering function was also described by Zimm mode in a short-time region, suggesting that the gel behaves like the sol. However, in a long-time region, the data points deviated from Zimm function, suggesting that the long-time dynamics was restricted by the cross-links.

Mesomorphic Phase Formation of Isotactic Polypropylene

It is well known that isotactic polypropylene (iPP) forms an intermediate structure between crystal and amorphous when molten iPP is rapidly quenched below 0°C. The structure is referred to as “mesomorphic phase”. The term has sometimes been used to describe structures of highly imperfect crystals. However, this is not relevant to the mesomorphic phase of iPP. Only iPP with high tacticity (iPP-HT) can form the mesomorphic phase by the rapid quench, whereas iPP with low tacticity (iPP-LT) cannot form the mesomorphic phase but it crystallizes by the same rapid quench (Fig. 3a). If the mesomorphic phase related to the imperfectness of crystal, the decrease of tacticity should enhance the formation of the mesomorphic phase. What is the mesomorphic iPP? The mesomorphic iPP-HT shows longer regular 3/1 helices than the crystalline iPP-LT (Fig. 3b). The structure and its formation mechanism of the mesomorphic iPP are considered analogous to those of lyotropic liquid crystals since the long regular 3/1 helices should act as the mesogenic segments of liquid crystal. These results suggest that mesomorphic iPP is a liquid crystal like structure formed through a specific kinetic pass.

Figure 1. NSE spectrometer in JRR-3M reactor in Tokai.

Figure 2. Scattering intensities of the first gel measured by SANS-U ( ) and NSE ( ) spectrometers. The intensity by NSE is divided into the static ( ) and dynamic ( ) fluctuations.

Figure 3. Wide angle X-ray diffraction profiles (a) and Fourier transform infrared spectra (b) of crystallized iPP-HT (black line), the quenched iPP-HT (red line) and the quenched iPP-LT (blue line). n: minimal number of 3/1 helical sequence.


Division of Multidisciplinary Chemistry  
- Molecular Rheology -

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

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Prof CHHABRA, Raj P.  Indian Institute of Technology, 6 July 2004

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

Research Activities (Year 2004)

Presentations
Detailed Investigation of Entanglement Dynamics with Dielectric and Viscoelastic Methods, Watanabe H, Annual APS March Meeting, Montreal, Canada, 22 - 26 March.
Nonlinear Rheology of Detergent Solutions, Inoue T, Annual Meeting of the Society of Rheology Japan, Tokyo, 13 - 14 May.
Viscoelastic and dielectric behavior of entangled blends of linear polyisoprenes: test of tube dilution picture, Watanabe H, The XIVth International Congress on Rheology, Seoul, Korea, 22 - 27 August.
Nonlinear rheology of aqueous detergent solutions, Inoue T, XIVth International Congress on Rheology, Seoul, Korea, 22 - 27 August.
Rheo-dielectric behavior of poly(ethylene oxide) containing lithium perchlorate, Matsumiya Y, The XIVth International Congress on Rheology, Seoul, Korea, 22 - 27 August.
Electric Birefringence of Poly(Propylene Glycol), Kikuchi T, the Discussion Meeting of the Society of Rheology Japan, Hiroaki, 22 - 24 September.
Dielectric Relaxation and Rheology of Lithium Per-
Orientational Anisotropy for Rouse Eigenmodes during Creep and Recovery Processes

The Rouse model is a fundamental molecular model for polymer dynamics and its dynamic behavior under step strain has been fully analyzed in literature [1]. However, surprisingly, no analysis has been made for the orientational anisotropy of the Rouse eigenmodes during the creep and recovery processes. For completeness of the analysis of the model, this anisotropy is calculated from the Rouse equation of motion [2].

The calculation, conducted with the Laplace inversion method on the basis of the pole analysis, is simple and straightforward. However, the result is intriguing in a sense that the anisotropy amplitudes $A_p$ of the Rouse eigenmodes during the creep/recovery processes are mutually correlated with each other because of the constant stress requirement. For $A_p$ of the higher order eigenmodes with $p \geq 2$, this correlation results in prominent overshoot and undershoot (to negative values) during the creep and recovery processes, respectively (see Figure 1). Correspondingly, each Rouse eigenmode has a distribution in the retardation time. These features are quite different from those under strain-controlled relaxation/flow processes where each eigenmode is associated with a single characteristic time and thus the modes behave independently to have monotonically growing/decaying anisotropy amplitudes.


Linear Viscoelastic Behavior of Perfluorooctyl Sulfonate Micelles: Role of Cations

Rheological behavior of threadlike micelles of anionic surfactants has been a subject of extensive research [1]. Nevertheless, the role of counter cation in this behavior has not been fully elucidated. This role was examined for a series of aqueous solutions of perfluorooctyl sulfonate (C8F17SO3⁻; FOS) micelles having a mixture of tetraethylammonium (N⁺(C2H5)4; TEA) and tetramethylammonium (N⁺(CH3)4; TMA) ions as the counter cations [2]. The solutions had the same FOS concentration (0.045 mol L⁻¹) and various TEA fraction in the counter cations, $\phi_{\text{TEA}} = 0 - 1$, and the spherical FOS micelles therein were connected into threads and further organized into dendritic networks.

For $\phi_{\text{TEA}} \geq 0.5$, the FOS threads/networks exhibited the Maxwell-type terminal relaxation reflecting their thermal scission. In this range of $\phi_{\text{TEA}}$, the terminal relaxation time $\tau$ drastically increased with decreasing $\phi_{\text{TEA}}$ (see Figure 2). On a further decrease of $\phi_{\text{TEA}}$ below 0.3, $\tau$ became insensitive to $\phi_{\text{TEA}}$, possibly because the motion of the threads in the unscissored form became faster than the thermal scission to govern the terminal relaxation.

These rheological features reflected the effects of TEA and TMA on the thermal scission of the FOS threads/networks: Since the charge was the same for TEA and TMA but the bare radius was smaller for TMA, the TMA cations should be preferentially bound on the FOS thread. The thermal scission of the FOS thread, occurring through an exchange of the bound and non-bound TEA cations [3], appeared to be strongly suppressed by the preferentially bound TMA cations that effectively blocked the exchanging sites. Indeed, in a range of $\phi_{\text{TEA}} \geq 0.5$ where the thermal scission governed the relaxation of the system, the rheological data were well described by a simple model considering this blocking effect (solid curve in Figure).


chlorate/Poly(Ethylene Oxide) System, Matsumiya Y, the Discussion Meeting of the Society of Rheology Japan, Hirosaki, 22 - 24 September.

Partial Tube Dilation in Entangled Binary Blends, Watanabe H, the Discussion Meeting of the Society of Rheology Japan, Hirosaki, 22 - 24 September.
Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

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

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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 microparticles, bionanoparticles, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2004)

Presentations
Dielectric Properties of Membranes, Asami K, 26th Annual Meeting of the Membrane Society of Japan (Tokyo, Japan), 20 - 21 May.


Electronic Structure of 2,5-Diarylsilole Derivative Thin Films Studied with Ultraviolet Photoemission and Inverse Photoemission Spectroscopies, Sato N, Yamagami T, Yoshida H, Yamaguchi S (Nagoya U.), Tamak K, Uchida M (Chiao Co.), The 8th Japan-China Joint Symposium on Conduction and Photo-conduction in Organic Solids and Related Phenomena (Okazaki, Japan), 11 - 14 November.

Dielectric Relaxation of a Nonionic Microemulsion during the Temperature-dependent Phase Inversion, Asami K, Membrane Symposium ’04 (Kyoto, Japan), 18 - 19 November.

Grants

Yoshida H, Controlling Reactivity and Diffusion at Metal-Organic Semiconductor Interfaces through the Deposition of Metal Clusters, Grant-in-Aid for Scientific Research for Young Scientists (B), 19 October 2004 - 31 March 2006.
Study of Thin Films of Carrier-doped Strontium Titanate with Emphasis on Their Interfaces with Organic Thin Films

Carrier-doped strontium titanate (M:STO, M = V, La) thin films prepared epitaxially on single crystalline strontium titanate (STO) substrates with the pulsed laser deposition method turned out to have surface flatness, surface electric conductivities and work functions no less useful for optically transparent anode materials of organic optoelectronic devices, e.g., organic light emitting diodes in the typical architecture, than indium tin oxides (ITOs). Whereas their optical transmittance is not high enough to employ for such use at this moment, further developments on this aspect are to be expected. Among the studied STO thin films V:STO is noted for its distinguished properties. The physical properties of M:STOs appear to depend on the site of atomic substitution involving charge carrier doping in their perovskite structures, which suggests that further optimization of dopant atoms and doping levels will lead to a transparent anode material with much higher performance. The observed difference in interfacial behaviors of energy levels of copper phthalocyanine (CuPc) overlayers between V:STO and ITOs using ultraviolet photoemission spectroscopy, that is, monotonous energy decreases of both the hole conduction level and the vacuum level with increasing thickness observed for an CuPc overlayer only on V:STO (see Figure 1), seems to demonstrate the effect by higher surface flatness of the V:STO substrate. On the very flat surface the molecular orientational change depending on the layer thickness will be expected and such a behavior may cause the monotonous change of the energy levels mentioned above. Finally, this work was carried out in collaboration with Professor Takano’s group.

Dielectric Study on Phase Inversion in Microemulsions

Microemulsions are apparently homogeneous mixtures including at least water, oil and surfactant. Some of them show temperature-dependent phase inversion, i.e., the type of emulsions inverts around the temperature at which bicontinuous structure appears, as schematically depicted in Figure 2. The phenomenon that is related to percolation is particularly interesting in view of the dielectric study of heterogeneous systems. In this report, the phase inversion in a ternary mixture of water (10 mM KCl), toluene and Triton X-100 (40: 40: 20 wt %) has been studied by dielectric spectroscopy over a frequency range of 10 Hz to 1 GHz. The transition from the water-in-oil type emulsion to the bicontinuous phase provided maxima for the intensity and the relaxation time of dielectric relaxation, which was accompanied with a steep increase in low-frequency conductivity. The characteristics of the dielectric behavior have been accounted for by interfacial polarization with a percolation model in which spherical water droplets are randomly connected with their nearest neighbors using water bonds.

Figure 2. Temperature-dependent phase inversion of microemulsion.

Figure 1. Thickness dependence of the apparent vacuum level and the valence level of CuPc overlayers on a V:STO film substrate. The upper panel: vacuum level with reference to that of V:STO, the lower panel: valence level with reference to its Fermi level.

Figure 3. Dr. Rainer Friedlein from Linköping University, Sweden, gave a fascinating seminar.
Scope of Research

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

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

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

Research Activities (Year 2004)

Presentations


Regulation of membrane lipid dynamics in cell polarization. Umeda, M. 45th International Conference on the Bioscience of Lipids. 25 - 29 May, Ioannina Greece.

Role of membrane lipids in regulating the thermoregulatory behavior of Drosophila. Umeda, M. Advanced Research Symposium on Drosophila. 31 May, Kyoto.


Grants


Regulation of Membrane Phospholipid Dynamics and its Role in Cell Morphogenesis

Biomembranes consist of a lipid bilayer whose major components are phospholipids. Although it is well known that phospholipids are distributed between the inner and outer leaflets of the bilayer membrane, mechanisms underlying the regulation and/or maintenance of this asymmetry are still poorly understood. To investigate the molecular mechanisms, we have isolated a series of yeast mutants with disordered organization of membrane phospholipids. By analyzing the genes defective in these mutants, we have identified a novel membrane protein, Ros3p, required for the translocation of phospholipids across the yeast plasma membrane. Studies using genetic manipulations of the Ros3p expression revealed that Ros3p protein is also involved in the regulation of cell morphogenesis via organizing actin cytoskeleton and cell polarity.

Ros3p is highly conserved among various organisms including worm, fly and mammals. Recently we have cloned a fly Ros3p homolog gene, dROS3, and created loss-of-function flies using RNA-mediated gene interference (RNAi) technique. The reduced expression of dROS3 protein caused marked reduction in body size and lethality at the pupal stage. Further analyses showed that the suppression of dROS3 protein expression also caused remarkable reduction in the size of fat body cells, implying a role of dROS3 in the regulation of cell size (Figure 1). These results suggest that ROS3 family acts as a multifunctional protein regulating both the membrane phospholipid organization and the cell morphogenesis.

Stearoyl-CoA Desaturase in Drosophila: Thermoregulation and Energy Metabolism

Stearoyl-CoA desaturase is the rate-limiting enzyme in the biosynthesis of monounsaturated fatty acids. It catalyzes the introduction of the cis double bond in the Δ9 position of fatty acyl-CoA substrates (Figure 2). The ratio of unsaturated/saturated fatty acids is one of factors influencing cell membrane fluidity, which determines temperature responses of ectothermal animals.

To investigate the action of desat1, which is the ortholog of mammalian stearoyl-CoA desaturase in thermoregulation of Drosophila, we generated the hypomorphic allele desat1/42 by mobilizing P element in desat1 locus. Genetic analyses revealed that desat1/42 allele lacks both of the third and fourth exons in 5’-flanking region of the desat1 gene. Immunohistochemical analyses showed that desat1 was widely expressed in brain, gut, fat body, and oenocyte of the wild-type flies. Although we detected no difference of the expression profile of desat1 in brain, gut, and fat body between wild type and the desat1/42 mutant, the expression of desat1 in oenocyte was severely reduced in the desat1/42 mutant compared with wild type (Figure 3). The desat1/42 mutant cultured on a fatty acid-free defined medium also showed a dramatic reduction in body weight and reduced triglyceride storage in fat body (Figure 4). The desat1/42 mutant will provide a unique model for studying the physiological functions of desat1 in energy metabolism as well as thermoregulation of Drosophila.

Figure 1. Suppression of dROS3 expression resulted in decreased cell and body sizes.

(a) Body size of third instar larvae of the wild type and the dROS3 reduced line.
(b) Nuclei of fat body cells in the wild type and the dROS3 reduced line were stained with DAPI. Sizes of each cell and nucleus in the dROS3 reduced line are smaller than those in the wild type.

Figure 2. Oxidative desaturation of fatty acids by stearoyl-CoA desaturase.

Figure 3. Patterns of expression of desat1 in embryonic oenocyte. Oenocyte (arrows) in wild type and the desat1/42 mutant were immunostained with polyclonal antibodies raised against desat1 protein (red) and neuron-specific monoclonal antibody (green). Scale bars: 10 μm.

Figure 4. Body weight of male and female wild-type and the desat1/42 mutant flies cultured on a fatty-acid-free defined medium.
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 2004)

Presentations
Electron Cooling System of Hot Ion Beam at S-LSR

Electron cooler for S-LSR is designed to cool down the laser produced ion beam with the rather large energy spread of the order of ±1% after phase rotation. It is to be installed in a straight section 1.86 m in length. In Fig. 1, the cross-sectional view of the electron cooling system is shown. So as to realize a compact size, the radius of curvature of the toroid determined to be 0.25 m and an elliptical shape of drift tube is adopted. Up to now, all the electron coolers ever used have utilized a circular shape for the drift tube and it is anticipated that the effect of space charge caused by the electron beam is not uniform. Such effect, however, is expected to be well manageable by the computer simulation. In order to realize efficient cooling rate, it is required that the temperature of the electron beam is as low as possible. As the electron is accelerated by the high voltage up to 5 kV after emission from the gun cathode, the longitudinal temperature of the electron beam is damped, but the transverse temperature remains as the value when it is emitted. So as to manage this situation, scheme to realize adiabatic expansion has been applied. For such a purpose, the magnetic field of the solenoid has been decreased from 1.5 kG at the gun region to 0.5 kG at the central cooler region. By such an expansion of factor 3, the transverse temperature of the electron beam has been decreased from 120 meV (1400 Kelvin) to 40 meV at the cooling region. With the above mentioned design, an electron cooling system has been constructed in 2004. In Fig. 2, the fabricated electron cooler is shown. The magnetic field has been evaluated with field measurement using Hall-probes. In order to keep the electron beam temperature to be low suppressing the temperature rise, it is needed to keep the uniformity of the magnetic field along the electron orbit. For such a purpose, correction coils are utilized at the transient regions between the solenoids and toroids, the effects of which has been evaluated by the field measurements and the results are indicated in Fig. 3. It is found that the homogeneity better than several x 10^-4 in the cooling region will be realized with careful adjustment of the excitation currents of the correction coils.

Figure 1. Cross-sectional view of the electron cooler for S-LSR.

Figure 2. Photograph of the fabricated electron cooler for S-LSR.

Figure 3. Improvement of the uniformity of the longitudinal field strength along the electron orbit with use of the correction coils attached at the transient regions between solenoids and toroids.


Grants


Scope of Research

The research subjects are ultra-intense and ultra-short laser-matter interactions and their applications. The physics of nano-contrabution and nano-structure formation on the surface of solid with short-pulse lasers are investigated, inquiring the new material science such as laser nano-processing and material creation. The process of ionization of large molecules and tissue with short pulse lasers is also studied to develop new mass spectrometers. With ultra-intense lasers, the physics of high energy electron generation and its applications are done research into. Ion generations by Coulomb explosion of molecules, clusters, and micro-particles, and sheath acceleration in thin foils and their applications to nuclear science are studied to open a new field of laser nuclear science. In the cooperation with the Laboratory of Electron Microscopy and Crystal Chemistry and the Laboratory of Structural Molecular Biology, the applications of laser produced electrons and x-rays to electron microscopy and x-ray analysis, respectively, will be studied. With the Laboratory of Particle Beam Science, new accelerator physics with laser-produced ions will be developed. For the applications of short pulse lasers to medicine, biological material, medical science and medical science we will collaborate with laboratories of this institute to challenge to develop a new field of interdisciplinary science. Main facility is the T6-laser (10TW, 100fs) available since 2004.

Presentations


Grants


Award

Completion of Laser Science Building for High Power Laser Facility in Advanced Research Center for Beam Science

To equip with ultra-intense femtosecond laser system T6-laser, a new laser building was completed adjacent to the building of accelerator facility. The laser building is constructed for less mechanical vibration on the floor against earthquake and high stability of temperature and humidity controls against muggy summer in Kyoto so that the laser system can be operated stably for long time. The building consists of a laser room and a laser-irradiation room. In 2004 fiscal year, the T6-laser system will be installed and be in operation. The part of laser irradiation experiment room will be opened for collaborators of ICR, Kyoto University, and other institutes. The T6-laser is named by the acronym of Table-top Ten TW Ten Hz Tunable Ti:sapphire laser. The system is Ti:sapphire chirped-pulse amplifier laser, delivering 1J (at maximum), 100fs pulses at a center wavelength of 800nm and repetition rate variable from single shot to 10Hz at maximum.

Energy Distributions of Ions Emitted from Argon Clusters Coulomb-exploded by Intense Femtosecond Laser Pulses

Energy distributions of ions emitted from argon clusters (up to 12 800 atoms/ cluster) Coulomb-exploded with an intense femtosecond laser have been experimentally studied. Under the laser intensity of 2x10^{16} W/cm^2, the ions of >15 keV are anisotropically emitted, while those lower than 15 keV tend to be isotropic. The argon ions of charge state up to Ar^{14+} were generated, and their high charge state is more than expected by the barrier suppression ionization model. The yield and maximum energy of Ar^{6+}-Ar^{14+} ions depend on laser polarization direction, while those of Ar^{6+}-Ar^{7+} are much less sensitive to the laser polarization. The present results suggest that high-charge-state and anisotropically emitted ions are produced by impact ionization of electrons that are produced by optical field ionization with the intense laser.

Periodic Structure of Metals with Femtosecond Laser Nano-Ablation

The laser ablation for Cu, Al, Fe, Zn, Ni, Pb, and Mo by short pulse laser (800 nm wavelength, 100 fs pulse duration, 1 kHz repetition rate) in air was studied. The craters produced by laser ablation were measured with a scanning electron microscope (SEM) and an atomic forced microscope (AFM). A periodic structure was observed at the bottom of the crater in all metals. The periodic structure was always oriented perpendicular to the electric field of laser polarization. A dependence of the periodic structure on the laser fluence was demonstrated in the range of 0.01-2 J/cm^2 for copper. The spacing d of the patterned structure was determined to be d = 300-40 nm for 0.07 J/cm^2 and d = 400-500 nm for 0.22 J/cm^2. As the laser fluence decreased, the spacing of the patterned structure had the tendency to be shorter. The formation of the periodic structure could not be explained by classical interference model. Some possible mechanisms in relation to the process of the periodic structure are discussed.

Desorption/ionization of Poly-aromatic Hydrocarbons with Intense Femtosecond Laser

Desorption/ionization of PAHs irradiated with intense femtosecond laser (800 nm wavelength, 100 fs pulse duration) was studied by means-of time-of-flight mass spectrometry. The molecular ions without heavy fragmentation was observed at the laser intensity around the ionization threshold. The signal intensity of the molecular ions increases with increasing the laser intensity. The ionization mechanism was suggested the non-resonant multiphoton ionization. The desorption/ionization with intense femtosecond laser will have a great possibility as a new soft-ionization method.
Advanced Research Center for Beam Science - Electron Microscopy and Crystal Chemistry -

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Prof CHOU, L-J National Tsing Hua University, Taiwan, 12 August 2004
Prof LAI, C-H National Tsing Hua University, Taiwan, 12 August 2004
Prof CHEN, H.-Z Zhejiang University, China, 15 November 2004

Scope of Research

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

Research Activities (Year 2004)

Presentations

Core Hole Effects on the Oxygen K-ELNES of Transition Metal Oxides, Kurata H, Tsujimoto M, Nemoto T, Isoda S, 8th APEM, 7 June.
Nanoscale Direction Control of 2-dimensional Organic Crystals at Liquid/solid Interface, Nemoto T, Takajo D, Kurata H, Isoda S, 8th APEM, 10 June.
Thin Film Structures and Optical Properties of the Bis(1,2-benzoxquinonenedioximato) Platinum(II), Yoshida K, Yaji T, Isoda S, EM-NANO 2004, 8 June.
Structures of Adsorbed Initial Layers of Stearic Acid at the Liquid/Solid Interface

The structures of stearic acid adsorbed initially on highly oriented pyrolytic graphite (HOPG) were examined at liquid/solid interfaces by scanning tunneling microscopy (STM). Depending on the concentrations of stearic acid in n-octylbenzene solutions, two structures were observed. For a saturated solution of stearic acid, the observed layer on HOPG was composed of large and stable domains under STM scanning, corresponding with the already reported structure (β-form). For low concentrations, molecular layers were also formed, but at the lowest concentration of 1.7 mM, the molecular layer became porous where an underlying layer with another structure (α-form) was observed. It was concluded that the α-form is the initially adsorbed layer and the second layer is formed as the β-form.

Takajo D et al., JAP, 43(7B), 4667 (2004).

Figure 1. STM images of the α- and β-form stearic acid on HOPG.

DV-Xα Calculation of Electron Energy-Loss Near-Edge Structures of F$_{4}$ TCNQ

The first principle molecular orbital (MO) calculations, focusing on the carbon K-edge fine structures, were performed for 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-quinodimethane (F$_{4}$TCNQ) and 7,7,8,8-tetracyanoquinodimethane (TCNQ). Electron energy-loss spectra (EELS) of F$_{4}$TCNQ were measured and analyzed through the calculation. In the discrete variational-Xα(DV-Xα) method, site-excited transition state configurations were assumed to take account of core-hole effects and, consequently, were examined in three parts: (1) partial density of states (PDOS) of unoccupied 2p orbitals; (2) inner 1s orbitals (energy-recalibrated PDOS); and (3) photo-absorption cross-section (PACS) considering the transition matrix. In F$_{4}$TCNQ, the inner 1s energy level of the quinoid-ring carbon combined to fluorine shifts deeper in energy, resulting in a high-energy shift of the π* peaks in the calculation. The calculation also showed the fluorescence effect on the quinoid-ring carbons appearing in the higher π* energy region. In the low energy region, the calculations accurately reproduced the core-excited spectra in both F$_{4}$TCNQ and TCNQ and succeeded in assigning each component appearing in the spectra.


Figure 2. Cryogenic electron spectro-microscope: STEM/TEM, Field emission gun, Liquid He cryo-holder, Ω-imaging filter, EELS, 2k×2k CCD detector.


Grants

Advanced Research Center for Beam Science  
- Structural Molecular Biology -

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

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Scope of Research

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

Research Activities (Year 2004)

Presentations


The relation between X-ray emission in LiNbO3 and its crystal structure, Ito Y, 18th International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, USA, 10 - 15 October (invited).

X-ray emission from pyroelectic crystal with the thermal process, Ito Y and Yoshikado S (Doshisha University), 60th workshop of the bulk growth in the Japanese Association for Crystal Growth Cooperation, Tokyo, Japan, 13 February (invited).

Grants

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

Structure-based Exploration of Functional Sites in the Aspartase Family

The crystal structure of the thermostable aspartase from *Bacillus* sp. YM55-1 was solved and refined for 2.5 Å resolution data. The enzyme is a homotetramer with subunits composed of three domains. It exhibits no allosteric effects, in contrast to the *E. coli* aspartase which is activated by divalent metal cation and L-aspartate. The overall folding of the present enzyme subunit is similar to those of the *E. coli* aspartase and the *E. coli* fumarase C, both of which belong to the same superfamily with the present enzyme.

In order to observe substantial structural differences in local sites, plots of the r.m.s. Cβ-deviation over five consecutive residues after Cα-fitting in this region between two structures are very effective. The local structural comparison of these three enzymes revealed seven structurally different regions (Figure 1).

Five of the regions were located around putative functional sites, suggesting the involvement of these regions into the functions characteristic of the enzymes.

Of these regions, the region of residues 96–100 is proposed as a part of the recognition site of the α-amino group in L-aspartate for aspartase and the hydroxyl group in L-malate for fumarase. The region of residues 315–323 is a flexible but well sequence-conserved loop that is suggested to be involved in the catalytic reaction. The region of residues 123–128 corresponds to a part of the putative activator-binding site in the *E. coli* fumarase C. The region in the *Bacillus* aspartase, however, adopts a main-chain conformation which prevents the activator binding. The regions of residues 228–241 and 265–272, which form a part of the active-site wall, are suggested to be involved in the allosteric activation of the *E. coli* aspartase by the binding of the metal ion and the activator.

![Figure 1. Overall structure of the active site that is formed by three subunits, A-, B-, and C-chains, which are colored green, blue, and red, respectively. Structurally different regions are colored yellow.](image)

Docking Model of the Substrate into the Active Site of the Aspartase

We have made a structural model of the complex in which a substrate L-aspartate was manually docked into the active site of *Bacillus* YM55-1 aspartase as follows (Figure 2).

The most conformationally different region in the vicinity of the active site is the region of residues 96–100, which is the sole region in which the structure of both the *Bacillus* aspartase and the *E. coli* aspartase differs from that of the *E. coli* fumarase. The amino acid sequence of the region is completely conserved among all aspartases, while partly different sequence is conserved for the corresponding region among all fumarases. Considering these findings and the characteristics of the functional groups bonding to the α-atom of substrates, we could expect this region to be the site recognizing the −NH₂⁺ group of L-aspartate in aspartase or the −OH group of L-malate in fumarase.

Because the substrates of aspartase and fumarase have two carboxyl groups as a common structural feature, positively charged residues have been suggested to stabilize these negatively charged groups. In the *Bacillus* aspartase, Lys524 is only one positively charged residue in the active-site cleft and the putative binding residue of one carboxylate of L-aspartate. The site of Ser140 and Thr141, which corresponds to one of binding sites for carboxyl group of the citrate in the citrate-fumarase complex, is just at the N-terminal end of α-helix 6. It is possible that the other carboxylate of the substrate bind to this site through the positively charged environment caused by the dipole moment of α-helix.

Finally, the substrate model was docked into the active site on the computer graphics so as to satisfy the proposals that the α-amino group may be recognized by Asp142, His188, and Gly98 or Thr101 and that the α- and β-carboxyl groups bind to Lys524 and Ser140 with the dipole moment of α-helix, respectively.

![Figure 2. The putative binding mode of substrate L-aspartate in the active site. The docked model of the substrate is represented by green bonds. Putative hydrogen bonds are shown by broken lines.](image)


Fujii T, Elucidation of mechanism of structural change in functional sites of aspartase, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.
International Research Center for Elements Science
- Organic Main Group Chemistry -

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Visitor
LI, Yongming
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SUN, Yedi (UG) University of Toronto, Canada, 10 May - 20 August 2004

Scope of Research

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

Research Activities (Year 2004)

Presentations
My Favorite Silicon and Boron (invited), Tamao K, Herbert C. Brown Lecture, 3 April, Purdue University, USA.
Palladium-Catalyzed Cross-Coupling Reaction of Aryltrimazenes with Organometallic Reagents, Sae Ki T, Son E-C, Matsunaga T, Tamao K, 51st Symposium on Organometallic Chemistry, 22 October, Tokyo, Japan.

Grants
Tsuji H, Development of New Method of Controlling Silicon Chain Conformation Aiming at Controlling Photophysical Properties of Oligosilanes, Grant-in-Aid for Young Scientists (B), April 2003 - March 2005.

Awards
Tamao K, Medal with Purple Ribbon, 29 April.
Tsuji H, Inoue Research Award for Young Scientists, Syntheses and Photophysical Properties of Oligosilane Conformationally Constrained by Methylene Tethers, Inoue Foundation for Science, 4 February.
Tsuji H, Progress Award in Silicon Chemistry, Japan.
The All-Anti Pentasilane

Recent studies have been unveiling the conformational dependence of the oligosilane σ conjugation: the anti conformation (SiSiSiSi dihedral angle ω = 180°) effectively extends the conjugation. For the highly conjugated system, it is desirable to control the silicon backbone precisely to anti. However, the peralkylated poly- and oligosilanes possess many kinds of conformers with smaller dihedral angles as energy minima, while the anti conformation corresponds to a local maximum on the energy surface. To overcome this problem, we have designed a bis(tetramethylene)-tethered bicyclic trisilane and prepared a pentasilane 1 with all-anti conformation.

The X-ray crystallography was performed on the diphenyl-substituted pentasilane as shown in Figure 1. The dihedral angles in the silicon backbone are 179.00(5)° and 179.11(5)°. The conformation of this compound is the closest to the ideal all-anti among the synthesized oligosilanes so far. UV absorption band of 1 corresponding to the lowest-energy σ-π* transition is much narrower at room temperature as compared with n- Si-Me12. The MCD of the pentasilane 1 show the characteristic signal to all anti conformation as well. These results demonstrate the effectiveness of the bicyclic trisilane unit for the conformation control in the silicon backbone.

![Figure 1.](image)

**Figure 1.** (a) Structure of all-anti pentasilane 1. (b) X-ray structure of the all-anti pentasilane derivative.


Cross-Coupling Reaction of 1-Aryltriazenes with Organotrifluorosilanes

We have recently reported that the cross-coupling reaction of 1-aryltriazenes with arenoboric acids readily proceeds in the presence of a palladium catalyst, a phosphine ligand, and a Lewis acid such as boron trifluoride (Scheme 1). The Lewis acid–base interaction between the boron trifluoride and the terminal nitrogen atom of the triazene might be essential to enhance the oxidative addition of the carbon–nitrogen bond to the zero-valent palladium complex.

![Scheme 1](image)

**Scheme 1.** Cross-coupling reaction of 1-aryltriazenes with arenoboric acids.

We have found a similar cross-coupling reaction with organosilicon compounds, instead of the boronic acids. Among the organosilicon compounds examined, only the most Lewis acidic trifluorosilane afforded the desired biaryl product. In this reaction, the addition of the external Lewis acid turned out not to be necessary, and finally the biaryl product was obtained in 76% yield (Scheme 2).

![Scheme 2](image)

**Scheme 2.** Cross-coupling reaction of 1-aryltriazene with trifluorosilane (plausible reaction mechanism).

The reaction system is applicable to the cross-coupling reaction with alkynyl-trifluorosilanes. As a typical example, the reaction of 1-(p-tolyl)triazene with (E)-styryltrifluorosilane readily proceeded at room temperature to afford the corresponding stilbene in 92% yield (Scheme 3).

![Scheme 3](image)

**Scheme 3.** Cross-coupling reaction of 1-(p-tolyl)triazene with (E)-styryltrifluorosi-
lane.

It is notable that the addition of methanol accelerates the coupling reaction in some cases. This effect is most remarkable for sterically hindered alkynyl silanes.

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Visitor  
Prof ETOURNEAU, Jean  
ICMCB-CNRS, France, 8 - 10 January 2004

Scope of Research

- Novel inorganic materials and devices that have new, useful or exotic features such as superconductivity, ferromagnetism and quantum spin ground state are synthesized and fabricated by novel methods. For example:
  - Oxides containing transition-metal ions in unusually high-valence state.
  - Nonequilibrium materials that can be obtained by high pressure method or epitaxial thin film deposition method.
  - Inorganic nanomaterials with useful functionality such as superparamagnetism and quantum size effect.

Research Activities (Year 2004)

Presentations

Fabrication and I-V Characteristics of pn Junctions Based on High Tc Superconductor Kao D, Terashima T, Shimakawa Y, Takano M, 11th International Workshop on Oxide Electronics, 3 - 5 October (Hakone).

Charge disproportionation of Ni(III) at the metal-insulator transition of RNiO3 (R = Pr, Nd), Saito T, Azuma M, Kanda H, Takano M, et al., 4th International Conference on Inorganic Materials, 19 - 21 September (Antwerp).


Grants


High Pressure Synthesis of Novel Cobalt Oxides and Their Magnetic and Transport Properties

We have found a novel cobalt oxide, SrCosO$_{11}$, by high pressure synthesis technique. As shown in figure 1, SrCosO$_{11}$ comprises Co$_3$O$_{10}$ Kagome layers with CoO$_6$ octahedra and CoO$_5$ bipyramids placed between them. Its spin system is geometrically frustrated, and has a strong spin-charge coupling, as seen in the sharp drop of the electrical resistivity when the spin structure is changed by external magnetic field. Such a spin-charge coupling via spin frustration has never been found so far, and is of keen interest. We are studying the detailed mechanism and the origin of the above physical properties, and are searching for new compounds with such a spin-charge coupling via spin frustration.

![Figure 1: Crystal structure of SrCosO$_{11}$ and the high pressure synthesis apparatus.](image)

Fabrication of Transition-metal Oxides p-(i)-n Heterojunctions by an Ion Beam Method

New type of heterojunctions comprising of YBa$_2$Cu$_3$O$_{6.8}$ (YBCO; p-type) and oxygen-deficient SrTiO$_3$ (STO; n-type) were fabricated by an Ar$^+$ ion beam method. Inset of Fig. 2 shows a schematical illustration of the junction: YBCO layer was grown on STO substrate by the pulsed laser deposition and a part of YBCO layer was etched by Ar$^+$ ion beam with a metal mask. n-type STO layer was generated by a slight reduction due to the relatively large sputtering rate of oxygen atoms in STO. Thus, p-(i)-n junction was formed at the interface between YBCO and STO layers. As shown in Fig. 2 the junction exhibits excellent rectifying current-voltage (I-V) characteristics, indicating that the method is of advantage for fabricating oxides p-(i)-n junctions. The interests of the junctions are a light emitting properties and a photovoltaic effect when the p and/or n layers are superconductive. Study for the junctions is now in progress.

![Figure 2: I-V characteristics for YBCO/STO p-n junction.](image)

Synthesis of Monodisperse, Submicron-Sized Spherical V$_2$O$_5$ Particles

Monodisperse, submicron-sized spherical metal oxide particles attract much interest in many areas of science and technology. We have succeeded in synthesizing monodisperse, submicron-sized spherical V$_2$O$_5$ particles with narrow size distribution via hydrolysis of a vanadium isopropoxide for the first time. Transmission electron microscopic observations revealed that the formed particles had almost perfect spherical shape and were non-agglomerated. V$_2$O$_5$ particles are possibly used in catalysis, lithium ion battery, electrochromic device, sensors and actuators. The monodisperse spherical V$_2$O$_5$ particles obtained by our developed method will greatly improve the performance in such applications.

![Figure 3: Transmission electron microscope image of V$_2$O$_5$ particles.](image)
Scope of Research

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

Research Activities (Year 2004)

Presentations
Catalytic C-O Bond Cleavage of Allylic Alcohols Using Diphosphinideneccyclobutene-Coordinated Palladium Complexes, Ozawa F, Murakami H, Ishiyama T, Yoshifuji M (Tohoku Univ.), The 14th International Symposium on Homogeneous Catalysis, 5 - 9 July, Munich, Germany.
Bromination of Four Acetylenic Protons on Cp'dFe(C=CH)2. Reactivity of the Resulting Bromoacetylene Fragments toward Nucleophiles, Okazaki M, Takano M (Tohoku Univ.), Ohtani T, (Tohoku Univ.) Tobita H (Tohoku Univ.), Ogino H (The Univ. of the Air), The 12th Japan-Korea Joint Symposium on Organometallic and Coordination Chemistry, 3 - 6 August, Sendai, Japan.
Stereocontrolled Synthesis and Photochemistry of cis-Poly(arylene vinylene), Katayama H, Nagao M, Nishimura T, Matsui Y, Nakamatsu K (Konan Univ.), Nawa H (Konan Univ.), Ozawa F, 50th Symposium of Organometallic Chemistry, Japan, 22 - 23 October, Tokyo, Japan.

Grants
Catalytic C-O Bond Cleavage of Allylic Alcohols and Ethers Using Diphosphinidenecyclobutene-Coordinated Palladium Complexes

We recently found that (π-allyl)palladium complex 1 bearing 1,2-bis(4-methoxyphenyl)-3,4-bis(2,4,6-tri-tert-butylphenylphosphinidene)cyclobutene (DPCB-OME) efficiently catalyzes direct conversion of allylic alcohols into N- and C-allylation products under mild conditions. In this study, we have elucidated a novel catalytic mechanism given in Scheme 1 [1]. Thus, unlike common allylation reactions involving oxidative addition of a C-O bond to a Pd(0) species, the C-O bond of allylic alcohols is cleaved by the action of hydridopalladium complex A. Proton-transfer from the Pd to the OH group in B, followed by elimination of water from C, forms π-allyl complex 1. We reasoned that strong π-accepting ability of DPCB-OME ligand as an sp3-hybridized phosphorus compound efficiently stabilizes C as a Pd(0) species by π-back-donation to facilitate the proton-transfer in B.

This novel catalysis is applied to deallylation of a variety of allyl ethers in aniline to give corresponding alcohols in high yields under mild conditions (Scheme 2) [2]. The reactions can be performed in air without loss of a variety of functionalities including vinyl, alkynyl, hydroxy, acetoxy, silyloxy, and acetal groups.

Reversible Cleavage and Recombination of Acetylenic Carbon-Carbon Bond on a Tetran-iron Cluster Coupled with Two-Electron Redox Reaction

Two-electron reduction of 2 resulted in the coupling of two methyldyne ligands to afford 3 (Scheme 3) [3]. The point we wish to stress is that formation and cleavage of the carbon-carbon bond can be controlled on the Fe4 core by two-electron reduction and oxidation. Two-electron oxidation of 3 led to the cleavage of the carbon-carbon bond to reproduce 2. To our knowledge, our present study is the first example, in which the reversible carbon-carbon bond cleavage and formation occurs between acetylene and two methyldyne fragments via two-electron oxidation and reduction.

(Z)-Selective Cross-Dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinilideneruthenium Complexes

Vinylideneruthenium complex 4 serves as good catalyst precursors for (Z)-selective cross-dimerization between arylacetylenes and silylacetylenes in the presence of N-methylpyrrolidine (Scheme 4). The reactions proceed at room temperature to afford (Z)-1-aryl-4-silyl-1-buten-3-yne in over 90% regio- and stereo-selectivities. The resulting enynes are efficiently desilylated by treatment with K2CO3 in MeOH to give terminal alkenylacetylenes (ArCH=CH-C≡CH) with (Z)-configurations.


Award
Ozawa F, The BCSJ Award, Insertion of Phenylacetylene into [Pt(GeMe)(SnMe)(PMe3Ph)2], The Chemical Society of Japan, 15 July 2004.
Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-scale materials and to develop opto-nanoscience for creation of innovative functional materials. Optical responses of semiconductor quantum nanostructures and low-dimensional strongly correlated electron systems are studied by means of space- and time-resolved laser spectroscopy. The main subjects are as follows: (1) Development of high-resolution scanning near-field optical microscope and optical properties of single nanostructures, (2) Ultrafast optical spectroscopy of excited states of semiconductor nanostructures, and (3) Development of nanoparticles with new optical functions.

Research Activities (Year 2004)

Presentations

Luminescence from Single Nanoparticle Phosphors (Special Lecture), Kanemitsu Y, The 71st Meeting of The Electrochemical Society of Japan, 24 - 26 March, Yokohama, Japan.


Grants


Inouye H, Luminescence Dynamics of Nanoparticles in a Photonic Crystal and Study for Realizing High Luminescence Efficiency, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.
Single Nanoparticle Spectroscopy

Semiconductor nanoparticles of sizes comparable to or smaller than the exciton Bohr radius in bulk materials have attracted much attention, because they exhibit a wealth of quantum phenomena. We have prepared semiconductor nanoparticles embedded in dielectric matrices by many different techniques and discussed luminescence properties of single semiconductor nanoparticles studied by selective excitation spectroscopy and scanning near-field optical microscopy at low temperatures. The free-exciton and shallow-impurity luminescence show very narrow line widths. The deep impurity luminescence is broad even in single nanoparticles. We discussed the mechanism of the exciton-phonon coupling in semiconductor nanoparticles.

Optical Near-field Spectroscopy of Semiconductor Quantum Structures

Scanning near-field optical microscope with a spatial resolution of 100-150 nm (\(\lambda/7-\lambda/5\), \(\lambda\): wavelength of light) has contributed to explore novel electronic and optical properties of semiconductor quantum structures. Recently, the spatial resolution as high as 30 nm (\(\lambda/30\)) has been achieved by employing a specially designed fiber probe with a small and clear aperture in photoluminescence measurements of the semiconductor quantum structures. With using this advanced tool, we have demonstrated that the local optical probe directly maps out the center-of-mass wave function of an exciton confined in a GaAs quantum dot (Fig. 2). The photoluminescence image in a biexciton (bounded two-excitions due to Coulomb interactions) state differs from that in an exciton state due to different distributions of the polarization field for the exciton and biexciton recombinations.

Femtosecond Laser Spectroscopy of Wide Band-Gap Semiconductors

Recently, there has been great interest in the optical processes in wide-gap semiconductors. The developments of wavelength-tunable femtosecond laser systems and remarkable progress in semiconductor crystal growth have enabled us to study intrinsic optical processes and dynamics. Because of the large exciton binding energy, GaN and related materials provide us an excellent stage for the study of the excitonic many-body effects in semiconductors. We have clarified the luminescence processes in highly excited GaN and InGaN semiconductors by means of optical Kerr-gate time-resolved photoluminescence measurements (Fig. 1).

Figure 1. Schematic of optical Kerr-gate time-resolved photoluminescence measurements using femtosecond laser pulses.

Figure 2. Exciton wave function image in a GaAs quantum dot by near-field photoluminescence mapping.

Awards


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

Research Activities (Year 2004)

Grants
Kanehisa M, Biological systems database (KEGG) and genome information science. Research for the Future Program, JSPS.
Kanehisa M, BRITE: Deductive Database of the Genome and the Biological System Based on Binary Relations, Bioinformatics Research and Development, JST.
Kanehisa M, Education and Research Organization for Genome Information Science, MEXT.
Kanehisa M, Knowledge Information Infrastructure for Genome Science. Kyoto University 21st Century COE Program, MEXT.
**KEGG GLYCAN: Computational Approach to Comparative Glycomics**

Glycans are an important class of biological macromolecules in addition to DNA and proteins. Under the KEGG project we released the GLYCAN database for carbohydrate structures and its associated information (Figure 1). We developed a novel method for conducting comprehensive analyses of comparative glycomics using glycan structures in KEGG GLYCAN. First, we developed a new similarity measure for comparing glycan structures taking into account the characteristic mechanisms of glycan biosynthesis, and we applied it to classify glycans of different species and tissues in the framework of support vector machines (SVMs). Next, we extracted characteristic functional units (motifs) of glycans (Figure 2).

![Figure 1. Structure based glycan database, KEGG GLYCAN.](image1)

![Figure 2. Extracted characteristic glycan structure of mouse.](image2)

**KEGG Orthology: a Hierarchical Classification of All Functional Orthologs in the Gene Universe**

KEGG Orthology (KO) is developed from “Ortholog IDs”, an extension of EC numbers in the KEGG PATHWAY database. It is one of the major projects of our laboratory and is intended to identify and classify orthologous gene clusters among all species stored in the KEGG GENES database. Using the KEGG SSDB database, orthologs in the KEGG GENES database are classified and annotated both automatically and manually. Namely, orthologs are classified by a computational clustering method according to KEGG SSDB scores (Figure 3), and the function of each ortholog is further examined manually.

![Figure 3. Ortholog Cluster Viewer on KEGG SSDB.](image3)

Many genome sequencing projects for eukaryotes are ongoing, and many draft genomes are available. Despite the delays in completing the genome project for eukaryotes, the draft sequences provide much important information. Therefore, the DGENES database was added to the KEGG database in order to store such draft genomes (Figure 4). We are currently developing automatic methods to annotate the genes in DGENES according to the KEGG Orthology.

![Figure 4. KEGG DGENES database.](image4)

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

Goto S, Construction and retrieval of highly integrated biological databases. Grant-in-Aid for Scientific Research on Priority Areas “Genome Information Science”, MEXT.
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Dr. VERT, Jean-Philippe
Mr. MAHÉ, Pierre

The University of Hong Kong, 2 September - 29 October 2004
The University of Hong Kong, 21 October 2004
The University of Hong Kong, 21 October 2004
Ecole des Mines de Paris, 4 - 17 November 2004
Ecole des Mines de Paris, 27 November - 21 December 2004

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

Research Activities (Year 2004)

Presentations


Clusterizing of database sequences for fast homology search using upper bounds on alignment score, Ittoh M, Akutsu T, Kanohisa M, The 4th Int. Workshop on Bioinformatics and Systems Biology, 1 June.


Grants

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.
Analysis on Two Complementary Scale-free Networks

In a wide variety of real-world networks such as the World Wide Web and biological networks, the probability that a node with degree \( k \) (the number of edges connected to the node) appears in a graph is proportional to \( k^{-\gamma} \), where \( \gamma \) is a constant. Such a network is called a scale-free network with exponent \(-\gamma\), and metabolic pathways are an interesting instance of the scale-free networks which can be represented by each of two complementary networks. In one of the networks, each node corresponds to a chemical compound, and an edge between nodes represents a reaction from the chemical compound of one node to that of another node. In the other network, a reaction and an enzyme which catalyzes the reaction are placed at a node, and two nodes are connected when the same chemical compound appears in the reactions of the nodes. The latter network can be constructed with the line graph transformation (that is, an edge in the former network is transformed into a node) from the former network, but properties of networks generated with the line graph transformation were not well investigated.

We then showed that, given a scale-free network \( G \) with exponent \(-\gamma\), its transformed network \( L(G) \) is also a scale-free network with exponent \(-\gamma+1\). We also experimentally confirmed that \( L(H) \) formed a scale-free network, and its exponent was increased by the transformation, where \( H \) is a metabolic network stored in the KEGG database.

Figure 1. The distribution of the degree of nodes in the initial metabolic network from the KEGG database and its transformed networks.


Extensions of Graph Kernels for Classifying Chemical Compounds

Recent theoretical advances and experimental results have drawn considerable attention to the use of kernel methods in computational analysis and classification of data sets. The marginalized graph kernels have recently been proposed to measure a similarity between labeled graphs such as chemical compounds.

These graph kernels, however, are subject to several limitations. First, the marginalized graph kernels decompose a graph into an infinite set of possible paths based on a random walk model for computational efficiency. This may lose structural information of graphs such as subtrees and subgraphs, which can be more relevant features in classification than paths. Moreover, the random walk model sometimes generates paths in which it comes to a node and instantly goes back to its previous node. Such a path only holds information on a local structure of the decomposed graph. Second, the marginalized graph kernel requires much computational cost, which results in slow implementation for real-world problems.

We then proposed two extensions of the marginalized graph kernels, which try to address these issues. The first extension is to relabel each node automatically in order to insert information about the environment of each vertex in its label by an iterative process called the Morgan index. This is effective in terms of feature relevance, because label paths contain information about their environment as well, and computation time, because less number of labeled paths match between graphs. Second, we showed how to modify the random walk model in order to remove irrelevant paths. Each method was validated on benchmark data sets, which are called the MUTAG and the PTC data sets, of classification of chemical compounds.

Figure 2. Computation time using different number of iterations of the Morgan index for the MUTAG and PTC data sets.


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

The mission of proteome informatics is to develop information technologies to draw a picture of the complicated relationships among biological components, mainly proteins, from a vast amount of accumulated biological data. The objective of this laboratory is to undergo research to develop new technologies based on computer science that tackle a variety of issues in proteome informatics, and consequently, to acquire new biological knowledge that contributes to molecular biology as well as pharmacology and the medical sciences. Our particular emphasis has been placed on the following three topics: 1) new probabilistic models and methods for estimating parameters for learning/mining, 2) new efficient algorithms for searching similar chemical compounds, and 3) new methods and models for matching and aligning glycans based on statistical techniques.

Research Activities (Year 2004)

Presentations

Application of Machine Learning to Bioinformatics, Mamitsuka H, Summer School of Bioinformatics (Spon- cered by Japanese Society of Bioinformatics), Wajima, Japan, 21 July.

Application of a New Probabilistic Model for Recognizing Complex Patterns in Glycans, Aoki K F et al., 12th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2004), Glasgow, UK, 3 August.


Grant
Mining and Predicting Protein-Protein Interactions

Protein-protein interactions play a number of central roles in many cellular functions, including DNA replication, transcription and translation, signal transduction and metabolic pathways. A recent increase in the number of protein-protein interactions has made predicting unknown protein-protein interactions important for the understanding of living cells. However, the protein-protein interactions experimentally obtained so far are often incomplete and contradictory, and consequently existing computational prediction methods have integrated evidence (latent knowledge of proteins) from different and more reliable sources. Analyzing the relationships between proteins and the latent knowledge is important to understanding the cellular processes. For this analysis, we have proposed a new probabilistic model for protein-protein interactions by considering the latent knowledge of proteins. We have further presented an efficient learning algorithm for this model, based on an EM (Expectation-Maximization) algorithm. Experimental results have shown that in a supervised test setting, the proposed method outperformed five other competing methods by a statistically significant factor in all cases. Using the probability parameters of a trained model, we have further shown the latent knowledge that is essential to predicting protein-protein interactions. Overall, our experimental results confirmed that the proposed model is especially effective for analyzing protein-protein interactions from a viewpoint of the latent knowledge of proteins.

Managing and Analyzing Carbohydrate Data

One of the most vital molecules in multicellular organisms is the carbohydrate, as it is structurally important in the construction of such organisms. In fact, all cells in nature carry carbohydrate sugar chains, or glycans, that help modulate various cell-cell events for the development of the organism. Unfortunately, informatics research on glycans has been slow in comparison to DNA and proteins, largely due to difficulties in the biological analysis of glycan structures. Our work consists of data engineering approaches in order to glean some understanding of the current glycan data that is publicly available. In particular, by modeling glycans as labeled unordered trees, we have implemented a tree-matching algorithm for measuring tree similarity. Our algorithm utilizes proven efficient methodologies in computer science that has been extended and developed for glycan data. Moreover, since glycans are recognized by various agents in multicellular organisms, in order to capture the patterns that might be recognized, we needed to somehow capture the dependencies that seem to range beyond the directly connected nodes in a tree. Therefore, by defining glycans as labeled ordered trees, we were able to develop a new probabilistic tree model such that sibling patterns across a tree could be mined. In fact, we have developed a new algorithm for estimating the parameters of this model from given training data. The model and algorithm are the cutting edges even in computer science. We provide promising results from our methodologies that could prove useful for the future of glycome informatics.

Figure 1. Example of two interacting proteins and the latent knowledge (protein classes).

Figure 2. Common monosaccharide names, their abbreviations and symbols.

Figure 3. Example of multiple tree alignment obtained by the proposed probabilistic model.
Bioinformatics Center
- Bioinformatics Training Unit -

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

Prof TOH, Hiroyuki (D Sc)
Assoc Prof KUMA, Keiichi (D Sc)
Assist Prof DAIYASU, Hiromi (D Sc)
Assist Prof ICHIHARA, Hisako (D Sc)
PD KATOH, Kazuaka (D Sc)

PD HOSHIYAMA, Daisuke (D Sc)
PD YOKOI, Toshiro (D Agr)

Students
YAMAGUCHI, Takeshi (D5)  NEMOTO, Wataru (D2)
SATO, Tetsuya (D1)

Visitor
PILS, Birgit
Department of Bioinformatics, Wurzburg University, Germany,
6 July - 22 August 2004

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 2004)

Presentations
Prediction of Interfaces for the class A GPCR oligomerization, Nemoto W, Toh H, 1st Pacific-Rim International Conference on Protein Science, 15 April.
Investigation of the cause of rate reduction observed in higher vertebrates, Hoshiyama D, Kuma K, Toh H, Miyata T (JT Biohistory Research Hall, Waseda University), Society of Evolutionary Studies, Japan 6th Annual Meeting, 6 August.
Molecular evolution of polar lipid biosynthesis in Archaia, Toh H, Yokoi T, Daiyasu H, 27th The Molecular Biology Society of Japan, 8 December.
Estimation of divergence time between Chlorella and land plants, and molecular evolution of Chlorella TPI
Basal Jawed Vertebrate Phylogeny Inferred from Multiple Nuclear DNA-coded Genes

We have cloned and sequenced seven nuclear DNA-coded genes from 13 vertebrate species. These sequences, together with sequences available from databases including 13 jawed vertebrates from eight major groups (cartilaginous fishes, bichir, chondrosteans, gar, bowfin, telcost fishes, lungfishes and tetrapods) and an outgroup (a cyclostome and a lancelet), have been subjected to phylogenetic analyses based on the maximum likelihood method. Cartilaginous fishes have been inferred to be basal to other jawed vertebrates, which is consistent with the generally accepted view. The minimum log-likelihood difference between the maximum likelihood tree and trees not supporting the basal position of cartilaginous fishes is 18.3 ± 13.1. Our tree has also shown that living holosteans, comprising bowfin and gar, form a monophyletic group which is the sister group to telcost fishes. This is consistent with a formerly prevalent view of vertebrate classification, although inconsistent with both of the current morphology-based and mitochondrial sequence-based trees. Furthermore, the bichir has been shown to be the basal ray-finned fish. Tetrapods and lungfish have formed a monophyletic cluster in the tree inferred from the concatenated alignment, being consistent with the currently prevalent view. It also remains possible that tetrapods are more closely related to ray-finned fishes than to lungfishes.

Identification of Cryptochrome DASH from Vertebrates

A new type of cryptochrome, CRY-DASH, has been recently identified. The CRY-DASH proteins constitute the fifth subfamily of the photolyase/cryptochrome family. CRY-DASHs have been identified from Synechocystis sp. PCC 6803, Vibrio cholerae, and Arabidopsis thaliana. The Synechocystis CRY-DASH was the first cryptochrome identified from bacteria, and its biochemical features and tertiary structure have been extensively investigated. To determine how broadly the subfamily is distributed within living organisms, we searched for new CRY-DASH candidates within several databases. We found five sequences as new CRY-DASH candidates, which are derived from four marine bacteria and Neurospora crassa. We also found many CRY-DASH candidates from the EST databases, which included sequences from fish and amphibians. We cloned and sequenced the cDNAs of the zebrasfish and Xenopus laevis candidates, based on the EST sequences. The proteins encoded by the two genes were purified and characterized. Both proteins contained folate and flavin cofactors, and have a weak DNA photolyase activity. A phylogenetic analysis revealed that the seven candidates actually belong to the new type of cryptochrome subfamily. This is the first report of the CRY-DASH members from vertebrates and fungi.

Figure 1. The maximum likelihood tree inferred from the concatenated amino acid sequences (2,942 residues) of seven proteins.

Figure 2. Mapping of the residues corresponding to the invariant sites within the CRY-DASH subfamily on the Synechocystis CRY-DASH structure.

genes, Kuma K, Yokoi T (Hitachi, Ltd.), Harada Y (Hitachi, Ltd.), Mizoguchi T (Sun Chlorella Corp.), 27th The Molecular Biology Society of Japan, 10 December.

Prediction of Protein-Protein Interactions Based on Real-Valued Phylogenetic Profiles Using Partial Correlation Coefficient, Sato T, Yamanishi Y, Kaneshita M, Toh H, 15th International Conference on Genome Informatica, 13-14 December.

Grants


Award

VISITING PROFESSORS’ ACTIVITIES IN ICR
Laboratory of Molecular Rheology
Standing Corporate Auditor, Toyota Central R&D Labs, Inc
(41-1, Yokomichi, Nagakute, Nagakute-cho, Aichi-gun, Aichi 480-1192)

Lectures at ICR
1) Polymer-Clay Nanocomposite I
2) Polymer-Clay Nanocomposite II
3) High-Speed Technique for Climate Resistant Test of Coating by Using Hydrogen Peroxide Solution
4) Development and Application of Meso-Porous Materials I

Laboratory of Advanced Solid State Chemistry
General Manager, R&D Planning Department, Sumitomo Electric Industries, Ltd.
(1-3-12 Motoakasaka, Minato-ku, Tokyo 107-0051)

Lecture at ICR
Strategy in Research & Development at Sumitomo Electric Industries, Ltd.

Laboratory of Advanced Solid State Chemistry
Executive Director, Japan Science and Technology Agency
(4-1-8 Honmachi, Kawaguchi, Saitama 352-0012)

Vis Prof
KITAZAWA, Koichi
(Ph D)

Laboratory of Advanced Solid State Chemistry
Chairman and CEO, Renesas Technology Corporation
(2-4-1 Marunouchi, Chiyoda-ku, Tokyo 100-6334)

Lecture at ICR
Current status and Future of the Semiconductor Industry

Vis Prof
NAGASAWA, Koichi
(D Sc)

Laboratory of Advanced Solid State Chemistry (Foreign Guest Laboratory)
Professor, College of Chemistry, Peking University
(202 Chengfu Road, Haidian District, Beijing, 100871, China, P. R.)

Lecture at ICR
Rare Earth Separation and Functional Materials Chemistry

Vis Prof
YAN, Chun-hua
(Ph D)
Laboratory of Structural Organic Chemistry

Associate Professor, Institute for Advanced Research and Department of Chemistry, Graduate School of Science, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8602)

**Lecture at ICR**
Design of Acid-Base Interactions for Selective Organic Synthesis

---

Laboratory of Advanced Inorganic Synthesis

Senior Research Scientist, Kono low temperature laboratory, The Institute of Physical and Chemical Research (RIKEN)
(2-1, Hirosawa, Wako, Saitama 351-0198)

**Lecture at ICR**
Nano-science and nano-technology

---

Laboratory of Supramolecular Biology

PD, Howard Hughes Medical Institute, Department of Physiology and Biochemistry, University of California San Francisco
(Genetics Development and Behavioral Sciences Building, Room GD-481, 1550 4th Street, San Francisco, CA 94158, USA)

**Lecture at ICR**
Control of Dendritic Branching and Tiling by the Tricornered-Kinase/Furry Signaling Pathway in Drosophila Sensory Neurons

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Laboratory of Organotransition Metal Chemistry

Asia Liaison, Rolic Technologies Ltd.
(Mikatadai, Nishi-ku, Kobe 651-2277)

**Lecture at ICR**
Recent Progress and Applications of Orientation Technology for Liquid Crystals
Retirement

Professor SUGIURA, Yukio
(Biofunctional Design-Chemistry,
Division of Biochemistry)

On the 31st of March 2005, Dr. Yukio Sugiura retired from Kyoto University after 40 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Sugiura was born in Kyoto on 3rd of February 1942. He graduated from Faculty of Pharmaceutical Sciences, Kyoto University in 1964. He studied metalllobiochemistry at the Graduate School of Pharmaceutical Sciences, Kyoto University, under the supervision of Professor H. Tanaka and was granted a doctoral degree for a thesis entitled “Correlation between Detoxication Activity of Heavy Metal Toxicity and Chelating Ability of Penicillamine” in 1971. In 1965, he was appointed as a Research Associate of the Laboratory of Radiopharmaceutical Chemistry, at the Graduate School of Pharmaceutical Sciences, Kyoto University. In 1982, he was promoted to an Associate professor of the Graduate School of Pharmaceutical Sciences, Kyoto University. In 1988, he was appointed as a full Professor of the Institute for Chemical Research, Kyoto University, and directed the Laboratory of Cancer Drug Research (present name: Laboratory of Biofunctional Design-Chemistry). He gave lectures at the Graduate School of Pharmaceutical Sciences, Kyoto University and supervised the dissertation works of graduate students.

During his academic carrier, Dr. Sugiura made a number of notable findings in wide area ranged from bioorganic chemistry, biomedical chemistry, and biofunctional chemistry, which he pioneered. He started research on the structure and function of bio-metal chromophores using the ESR techniques. Then he emerged his research to the molecular mechanisms of DNA cleavage by bleomycin and endiynyl antitumor antibiotics known by their strong antitumor activities. He firstly clarified the sequence- or conformation-specific DNA cleavage manners by endiynyl antitumor antibiotics including esperamicin, dynemicin, C-1027, and so on. For the recent years he investigated the mechanism of DNA recognition of the CysHisz-type zinc finger proteins and created a lot of artificial zinc finger proteins with novel DNA binding characteristics or hydrolytic ability. For these distinguished contributions to science, he was awarded the Pharmaceutical Society of Japan Award for Young Scientists in 1984, the Upjohn Scientific Research Award in 1992, and the Award of Pharmaceutical Society of Japan for the research entitled “Molecular Mechanism for DNA Recognition and Functional Expression of Bioactive Molecules” in 2000.

Dr. Sugiura also devoted himself to administration of Kyoto University as well as the Institute for Chemical Research, Kyoto University. He served as the Director at Institute for Chemical Research, Kyoto University and also as a senator of Kyoto University from 1998 to 2000. In 2000, he chaired the Kyoto University Uji Library. He greatly contributed to reorganization of journals and development of the electronic journals in the Kyoto University Library as a chairman of the committee for the library when he was a councilor for the library.

Dr. Sugiura contributed to various scientific societies. He served as a vice president of the Pharmaceutical Society of Japan during 2003 and 2005 and he is the present president of the society. Internationally, he was invited as a visiting professor by School of Pharmacy and Pharmaceutical Sciences, University of Manchester from 1998 to 2004. He organized as chairman the 5th AFMC International Medicinal Chemistry Symposium in 2003.

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

Professor UMEMURA, Junzo
(Solution and Interface Chemistry,
Division of Environmental Chemistry)

On the 31st of March 2005, Dr. Junzo Umemura retired from Kyoto University after 38-year service to Kyoto University. Dr. Umemura was born in Nagaike, Kyoto-ku on June 20, 1941. He graduated from the Department of Chemistry, Faculty of Science, Kyoto University in 1964. He studied vibrational spectroscopy in Graduate School of Science, Kyoto University under the supervision of the late Professor Rempei Gotoh. After completing his Master's Degree in 1966, he entered Nisui Chemical Industries in Nagoya to study physical properties of polymer films. In 1967, he was appointed as an Assistant Professor of the Institute for Chemical Research, Kyoto University. He continued his spectroscopic study in the group of Professor Tohru Takenaka and Associate Professor Soichi Hayashi to be granted a doctoral degree of Science, Kyoto University under the title of “Coexistence of Two Molecular Configurations in Crystalline Normal Fatty Acids as Studied by Infrared Spectra” in 1978. On leave from Kyoto University from 1978 to 1980, he studied structures of model biomembranes and aqueous micellar solutions by FT-IR spectroscopy under Dr. Henry H. Mantsch at the National Research Council of Canada in Ottawa as a Research Associate. He was promoted to an Associate Professor in 1994, and to a full Professor in 2003.

During his academic carrier, Dr. Umemura has devoted himself to the vibrational spectroscopic study of amphiphilic compounds that have both polar hydrophilic and non-polar hydrophobic groups within a molecule. He started his study from typical amphiphilic compounds of normal fatty acids in the crystalline state by performing low-temperature experiments down to liquid Helium temperature and normal coordinate analyses, giving decisive proof to the coexistence of two molecular configurations as a result of double proton transfers along two hydrogen bonds connecting two carboxylic groups of a dimer.

During his stay in Ottawa, two papers concerning the high-sensitive FT-IR monitoring of micelle formation of sodium alkanoates mark the first success by the IR method that had been believed to be difficult at the critical micelle concentration range owing to the strong absorption of water in the infrared region.

After coming back from NRCC, he started to investigate the Gibbs monolayer of a surface active azo dye adsorbed from its aqueous solution to the solution-CCL interface by resonance Raman spectroscopy. He found that in certain basic pH’s, the tautomeric structural change from the azo form to the protonated hydrazene form occurred upon adsorption. This was the first finding that the structure of adsorbed monolayer at the interface could be different from that in the aqueous solution. He also carried out FT-IR investigations of Langmuir films of insoluble monolayer on the water surface and Langmuir-Blodgett (LB) films of various amphiphiles transferred onto solid substrates. The layer-by-layer structure change of stearic acid LB films measured by the attenuated total reflection method [Langmuir, 2, 96 (1986)] attracted much attention in this field (290-time citation). He proposed a quantitative evaluation method of molecular orientation in LB films by comparing FT-IR transmission and reflection-absorption spectra [J. Phys. Chem., 94, 62 (1990)], and it is widely adopted for the characterization of LB films (270-time citation). Among his 132 original papers, seven are block-busters with more than 50 citations in any 7 years’ span.

He gave lectures on vibrational spectroscopy since 1994 at the Graduate School of Science, Kyoto University, and supervised the dissertation works of graduate students. He was a visiting lecturer at Kobe, Chiba, and Nagoya Universities, as well as Shiga University of Medical Science. He served as a member of the program committee of the Chemical Society of Japan. He also served as a member of the several international conferences on thin organic films.

His contribution to Kyoto University through both scientific and educational activities is hereby greatly acknowledged.
Early Retirement

Professor TAMAO, Kohei

(Organic Main Group Chemistry,
International Research Center for Elements Science)

On the 31st of March 2005, Dr. Kohei Tamao retired from Kyoto University one year earlier than the retirement age after 35 years of service to the university to move to RIKEN, Wako, Saitama.

Dr. Tamao was born in Kagawa on the 31st of October, 1942. He received his Bachelor of Engineering, Master of Engineering, and Doctor of Engineering from Kyoto University under the direction of Professor Makoto Kumada in 1961, 1967, and 1971, respectively. He was appointed as an Assistant Professor of Kumada laboratory, Department of Synthetic Chemistry, Faculty of Engineering, Kyoto University in 1970 and promoted to an Associate Professor of Professor Yoshihiko Ito’s group in 1987. He worked with J. J. Eisch, State University of New York at Binghamton, for one year from 1973 as a postdoctoral fellow. In 1993, he became a Full Professor at the Institute for Chemical Research, Kyoto University. He served the Institute as Director in 2000-2002 and the first Director of the International Research Center for Elements Science which was newly launched in the Institute in 2003.

He was also affiliated to the Division of Energy and Hydrocarbon, the Graduate School of Engineering, Kyoto University, to give lectures of organic chemistry course to graduate and undergraduate students.

His main research interests are organosilicon chemistry and transition metal catalyzed organic synthesis. In particular, he developed the nickel-phosphine catalyzed cross-coupling reaction between organic halides and organomagnesium reagents as a new carbon-carbon bond formation, which has opened up a new area in modern synthetic organic chemistry. This reaction is often called the “Kumada-Tamao-Corriu” reaction. The proposed catalytic cycle has been recognized as a prototype for many other transition metal catalyzed cross-coupling reactions. He was the first who demonstrated the synthetic applicability of hypercoordinate organosilicon compounds and later developed the oxidative cleavage of the silicon-carbon bond by hydrogen peroxide to form alcohols, which is now known as the “Tamao oxidation”. During the past decade, he also developed a new method for the synthesis of silicon-containing cyclic compounds, siloles, and applied them to electroluminescent devices as efficient electron-transporting materials, as well as the chemistry of functionalized silyl anions and oligosilane π-conjugated systems. Including these studies, he has published more than 230 original papers and 85 accounts, reviews and monographs.

Dr. Tamao received many honors, including the Chemical Society of Japan Award for young Chemists in 1977, the Chemical Society of Japan Award in 1999, the Toray Science & Technology Prize and the American Chemical Society F. S. Kipping Award in 2002, the Asahi Prize and the Mukai Prize in 2003, and Medal with Purple Ribbon in 2004.

Dr. Tamao was a research leader of the Kyoto University COE (Center of Excellence) “Elements Science” project, supported by Ministry of Education, Culture, Sports, Science, and Technology (MEXT) in 2000-2004. He is serving as the Vice President of the Chemical Society of Japan, the Editor-in-Chief of Bulletin of the Chemical Society of Japan, and the Chairman of The Society of Silicon Chemistry, Japan. He is also a member of several Councils for Science and Technology in MEXT. Dr. Tamao is now serving as Director of the Frontier Research System at RIKEN for the further development of academic research activities in Japan.

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

TAMAO, Kohei

Medal with Purple Ribbon

Great contribution to the scientific development through years of researches in organometallic chemistry, as represented by (1) the transition metal-catalyzed cross-coupling reaction between organomagnesium reagents and organic halides, (2) the hydrogen peroxide oxidation of the silicon-carbon bond, and (3) the synthesis and application of silole-containing π-conjugated systems.

29 April 2004

Herbert C. Brown Lecturer

“My Favorite Silicon and Boron”

3 April 2004

Medal with Purple Ribbon is awarded twice a year by the Emperor to some outstanding scientists and artists in respect of their creative, innovative or inventive contribution.

KAJIWARA, Takashi

The Best Oral Presentation Award

The 84th Annual Meeting of the Chemical Society Japan

“The First Generation of a Borylsilyl Anion and Its Trapping Reactions”

The Chemical Society of Japan

27 April 2004

SHINOHARA, Akihiro

The Best Oral Presentation Award

The 84th Annual Meeting of the Chemical Society Japan

“Reactions of a Kinetically Stabilized 9-Silaanthracene with Polycyclic Aromatic Hydrocarbons”

The Chemical Society of Japan

27 April 2004

The ICR Award for Students

“Synthesis of Kinetically Stabilized Silaaromatic Compounds and Their Properties”

ICR

3 December 2004
MURATA, Yasujiro

The Chemical Society of Japan Award for Young Chemists
“Novel Structural Transformation of Fullerene C60”
The Chemical Society of Japan
27 March 2004

ISHIDA, Shintaro

Inoue Research Award for Young Scientists
“Synthesis, Structure, and Reactions of the First Stable Dialkylsilylene and Trisilaallene”
Inoue Foundation for Science
4 February 2004

TSUBAKI, Kazunori

Kansai Branch Award
“Visualization of Molecular Properties using Functional Host Molecules”
The Society of Synthetic Organic Chemistry, Japan
19 November 2004

KUSUDA, Toshiyuki

Kyoto Prefecture Governor’s Award
Outstanding Leader in High Pressure Gas Production Safety Manager
26 October 2004

SAITO, Shigeki

The ICR Award for Students
“Arabidopsis CYP707A2 Encodes (+)-Abscisic Acid 8’-Hydroxylase, a Key Enzyme in the Oxidative Catabolism of Abscisic Acid”
ICR
3 December 2004

NAKAHARA, Masaru

Award of The Japan Society of High Pressure Science and Technology, 2004
“NMR Studies on Water and Aqueous Solution under High Pressure and Supercritical Conditions”
The Japan Society of High Pressure Science and Technology
10 October 2004
KURIHARA, Tatsuo

The Japan Bioscience, Biotechnology and Agrochemistry Society Award for the Encouragement of Young Scientists

“Bioconversion of Organohalogen Compounds with Microbial Enzymes: Mechanistic Analysis of the Enzyme Reactions and Their Application”

Japan Society for Bioscience, Biotechnology, and Agrochemistry

28 March 2004

NISHIDA, Koji

Promotive Award of the Society of Fiber Science and Technology, Japan, Kansai

“Control of Higher Order Structures of Polymer Materials by a Rapid Temperature Jump Method”

The Society of Fiber Science and Technology, Japan

8 December 2004

HASHIDA, Masaki

2003 LSJ Award for Distinguished Achievements in Research

“Femtosecond Laser Ablation of Metals: Characterization of New Processing Region and Formation of Nano-structures”

The Laser Society of Japan

28 May 2004

TSUJI, Hayato

Inoue Research Award for Young Scientists

“Syntheses and Photophysical Properties of Oligosilane Conformationally Constrained by Methylene Tethers”

Inoue Foundation for Science

4 February 2004

Progress Award in Silicon Chemistry, Japan

“Control of Conformation and Photophysical Properties of Oligosilanes Based on Bicyclic Structure”

The Society of Silicon Chemistry, Japan

29 October 2004

The ICR Award for Young Scientists

“Conformation Control of Oligosilanes Based on Bicyclic Structure”

ICR

3 December 2004

KANEMITSU, Yoshihiko

Phosphor Award

“Pioneering Contributions for Semiconductor Nanoparticles”

Phosphor Research Society, The Electrochemical Society of Japan

26 November 2004

INOUE, Hideyuki

Best Young Presenter Award

“Ultrafast Response of a Self-organized Closely-packed Metal Nanoparticles System”

Society of Nano Science and Technology

10 May 2004
TOII, Hiroyuki

The Okawa Publications Prize
“Bioinformatics for the Analysis of Protein Function”
Okawa Foundation

25 November 2004

Paper Awards

YAMAGUCHI, Akinobu1; TANIGAWA, Hironobu; ONO, Teruo;
NASU, Saburou1; MIYAKE, Kousaku2; MIBU, Ko3; SHINJO, Teruya4

MSJ Distinguished Paper Award
“Current-driven Domain Wall Motion Due to the Spin-transfer Effect”
Magnetics Society of Japan

22 September 2004

1 Osaka University, 2 Tohoku University, 3 Research Center for Low Temperature and Materials Science, Kyoto University, 4 International Institute for Advanced Studies

OZAWA, Fumiyuki, et al.

The BCSJ Award
“Inertion of Phenylacetylene into [Pt(GeMe)(SnMe)(PMe2Ph)3]”
The Chemical Society of Japan

15 July 2004
Poster Awards

SUGIYAMA, Yusuke

The Best Poster Award
The 17th Symposium on Fundamental Organic Chemistry
“Synthesis of a Dibromodigermene Derivative Utilizing Kinetic Stabilization and Its Properties”
The Committee of the 17th Symposium on Fundamental Organic Chemistry
25 September 2004

MAEDA, Shuhei

The Best Poster Award
The 17th Symposium on Fundamental Organic Chemistry
“Encapsulation of Molecular Hydrogen into an Open-Cage Fulleren C50 Derivative”
The Committee of the 17th Symposium on Fundamental Organic Chemistry
25 September 2004

MONGUCHI, Daiki

Best Poster Award
21st Summer School of Synthetic Organic Chemistry (Kyoto)
“Asymmetric Cyclization Based on Dynamic Chirality of Enolates”
The Society of Synthetic Organic Chemistry, Japan
14 July 2004

TANIMA, Daisuke

Best Poster Award
24th Seminar for the Young Researchers on Organic Synthesis
“Temperature-Dependent Colorimetric Chiral Recognition by Phenolphthalein Derivatives”
The Pharmaceutical Society of Japan (Kinki) and the Society of Synthetic Organic Chemistry, Japan (Kansai)
1 December 2004

INOUE, Rintaro

The Best Poster Award
UK-Japan Polymer Workshop
“Inelastic Neutron Scattering from Polystyrene Thin Films”
UK-Japan Polymer Workshop
1 April 2004

OGINO, Yoshiko

Poster Awards Second Prize
UK-Japan Polymer Workshop
“Crystallization of Isotactic Polypropylene under Shear Flow”
UK-Japan Polymer Workshop
1 April 2004
FUKAZAWA, Aiko

Symposium Poster Award
51st Symposium on Organometallic Chemistry, Japan
“Conformation Control of Oligosilanes Based on the Bis(tetramethylene)-Tethered Bicyclic Trisilane Unit”
Kinki Chemical Society, Japan
15 December 2004

OCHIAI, Tomoshiro
NACHER, Jose C.

Oxford University Press Bioinformatics Prize
The 15th International Conference on Genome Informatics, Japan
“Markov Property and Scale-free Organization of Gene Expression”
Japanese Society for Bioinformatics
15 December 2004
Obituary

Professor Emeritus
Dr. KUNICHIKA, Sango (1909-2004)

Dr. Sango Kunichika, Professor Emeritus of Kyoto University passed away on January 28, 2004 in Kyoto. Dr. Kunichika was born on February 18, 1909 in Hiroshima. In Hiroshima High School, his interest in organic chemistry was first excited. He graduated from the Department of Chemistry, Faculty of Science, Kyoto Imperial University in March, 1935. His first achievement was in the success of the synthesis of acetylformonoi under the direction of the late Professor Ryuzaburou Nodzu, Department of Chemistry, Faculty of Science. He was appointed a research assistant in April, 1935. He joined the Institute for Chemical Research, Kyoto University in May, 1938, and was appointed a lecturer in April, 1940, and an assistant professor in February, 1944. In September, 1948, he was conferred a D. Sc. from Kyoto University for his study on the synthesis of acetaldehyde from acetylene by the vapor phase method. For these years, he was concerned with the studies on reactivities of acetylene and its derivatives. In June, 1951, he was promoted to a full professor at Kyoto University. In the following years his interest was directed to the exploitation of new synthetic methods of various monomers and to the elucidation of the reactions used for the syntheses with many remarkable academic achievements.

Since 1955, Dr. Kunichika gave lectures on polymer chemistry at the graduate school of science, and supervised dissertation works of many graduate students. In 1965, he visited the United States to give a lecture on the new synthesis of methyl methacrylate from propylene at New York University.

For three years from December, 1964 to December, 1967 Dr. Kunichika served as Director of the Institute and above all contributed very much to the move of the Institute from Takedate to Uji. In December, 1970 he was nominated again as the Director, and he aided in the solution of many of problems until his retirement in March, 1972. He also showed his administrative ability as a member of the University Council and various committees on the campus. Further, he served as Director of the Kinki Area Chapter of the Chemical Society of Japan and that of the Society of Synthetic Organic Chemistry, Japan.

Owing to his sincere thoughtful and warm personality, Dr. Kunichika communicated well not only with the older member of the University but had a deep understanding with the students as well. His participation in student activities and his personal contact with the students helped to deepen this understanding. His motto was "to be deliberate in council and prompt in action." For these great academic and educational contribution Dr. Kunichika was awarded the Second Class Order of the Sacred Treasure in 1981.
Obituary

Professor Emeritus

Dr. KURATA, Michio (1925-2004)

Dr. Michio Kurata, Professor Emeritus of Kyoto University, passed away on September 10, 2004, in Kyoto.

Dr. Kurata was born on February 23, 1925 in Tokyo. In 1947, he graduated the Department of Applied Chemistry, Faculty of Engineering, Tokyo Institute of Technology and entered the Graduate School of Engineering in the same Institute. In 1948, he joined the Department of Industrial Chemistry, Faculty of Engineering, Kyoto University as a research student while keeping his position in Tokyo Institute of Technology. In 1952, he quitted Tokyo Institute of Technology and was appointed as a Lecturer in the Faculty of Engineering, Kyoto University. In 1954, he was appointed as an Associate Professor in the same Faculty. He got a Ph.D. (Doctor of Engineering) from Kyoto University in 1955. He stayed in USA as a Sloan Foreign Post-Doctoral Fellow at Massachusetts Institute of Technology from 1959 to 1960 and as a Research Associate at the same Institute and Dartmouth College from 1960 to 1961. In 1962, he was promoted to a full Professor of the Institute for Chemical Research, Kyoto University to direct the Laboratory of Polymer Solution (later reorganized to the Laboratory of Fundamental Material Properties, and presently, the Laboratory of Molecular Rheology, Division of Multidisciplinary Chemistry). In 1974, he spent two months in Sweden as a Nobel Guest Professor of Royal Academy of Sciences. He was appointed as the 21st director of the Institute for Chemical Research and a member of the University Council, Kyoto University from 1986 to 1988. He retired from Kyoto University in 1988, and was honored with the title of Professor Emeritus of Kyoto University. After the retirement, he served as an adviser for Mitsubishi Gas Chemical Company from 1988 to 1995.

Dr. Kurata contributed significantly to the progress in molecular understanding of physical properties of polymers in solutions and bulk. He was a pioneer in the research of dilute polymer solution properties and developed a statistical theory relating the intrinsic viscosity of the solution to molecular parameters of polymer chains. His theory motivated extensive experimental studies of dilute solutions that provided the basis of the current research field of dilute solutions. For polymers in concentrated solutions and bulk, he made extensive investigation of the nonlinear rheological properties and the chain dynamics. He utilized viscoelastic and optical methods backed up with detailed theoretical analyses to establish a molecular picture for the dynamics and relaxation of entangled polymer chains. His findings served as a basis for later development of the tube model theory for entangled chains. He extended his research to interactions of polymer chains and small molecules and revealed important effects of this interaction on transport phenomena such as the non-Fickian diffusion of the small molecules.

Dr. Kurata was a gentle and honest person. He educated many students and young scientists. He served as the Chief Editor of the Journal of the Society of Rheology, Japan from 1975-1979 and the President of this Society from 1985 to 1987. For his brilliant achievements in scientific and educational fields, Dr. Kurata was honored with the SPSJ Award for Outstanding Achievement in Polymer Science and Technology in 1988, Award of the Society of Rheology, Japan in 1990, and the Second Class of the Order of the Sacred Treasure in 2002.
Obituary

Assistant Professor

Dr. NAKAMATSU, Hirohide (1956-2004)

(Structural Molecular Biology,
Advanced Research Center for Beam Science)

Dr. Nakamatsu, Assistant Professor of Kyoto University, passed away on July 1, 2004 in Kyoto.

Dr. Nakamatsu was born on April 11, 1956 in Osaka. He graduated the Department of Chemistry, Faculty of Science, Osaka University in 1979 and entered the Graduate School of Science, Osaka University. After he got a Master of Science on Inorganic and Physical Chemistry from Osaka University, he was employed as a technician by the Institute for Scientific and Industrial Research, Osaka University. In 1989 he moved to the Institute for Chemical Research, Kyoto University and was appointed to an Assistant Professor of the Laboratory of Nuclear Radiation (presently, the Laboratory of Structural Molecular Biology, the Advanced Research Center for Beam Science). He got a Ph.D. (Doctor of Science) from Kyoto University in 1996.

His thesis was on the molecular orbital calculations of x-ray absorption spectra. From 1998 to 1999 he stayed at Northwestern University, Illinois, USA as a research fellow.

The work of Dr. Nakamatsu was mainly on the theoretical study of electronic structures of molecules by the use of the Discrete Variational Xα (DV-Xα) molecular orbital method. He extended this method for molecular excited states and calculated x-ray absorption spectra, especially x-ray absorption near-edge structure (XANES) for gases and solids. In order to produce the realistic potential in solids, he developed the chemically complete cluster method. His interest was also on the relativistic effects on electronic structures and he studied various molecules containing heavy elements using the relativistic DV-Xα method.

Dr. Nakamatsu served a Secretary and the member of the Steering Committee of the Society for Discrete Variational Xα from 1989. For his scientific achievements and contributions to the Society, he was awarded the Special Prize from the Society for Discrete Variation Xα in June, 2004.
DIVISION OF SYNTHETIC CHEMISTRY — Organoelement Chemistry —


— Structural Organic Chemistry —


— Synthetic Organic Chemistry —


[Others]


— Advanced Inorganic Synthesis —


[Others]


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--- Chemistry of Polymeric Functionalities ---


--- Inorganic Photonic Materials ---


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— Magnetic Materials —


DIVISION OF BIOCHEMISTRY — Biofunctional Design-Chemistry —


— Chemistry of Molecular Biocatalysts —


— Molecular Biology —


Molecular Clinical Chemistry

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DIVISION OF ENVIRONMENTAL CHEMISTRY
— Molecular Materials Chemistry —

Structure and Chain Conformation of Thermotropic Liquid Cryst-

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Studies of the Structure and Chain Conformation of Ther-
mothropic Liquid Crystalline Polyester Crystallized from the Liquid

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— Molecular Microbial Science —


**DIVISION OF MULTIDISCIPLINARY CHEMISTRY**

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**Molecular Rheology**


--- Supramolecular Biology ---


--- ADVANCED RESEARCH CENTER FOR BEAM SCIENCE ---

--- Particle Beam Science ---


--- Laser Matter Interaction Science ---


INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE
— Organic Main Group Chemistry —


— Advanced Solid State Chemistry —


--- ORGANOTRANSITION METAL CHEMISTRY ---


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[Others]


— Biological Information Network —


CONTRIBUTED CHAIR —

Proteome Informatics (SGI Japan) —


[Others]


**BIOINFORMATICS CENTER**

— Bioinformatics Training Unit —


[Others]


INTERNATIONAL RESEARCH COLLABORATIONS

[Austria]
Institute of Theoretical Physics, Graz University

[Belgium]
Electron Microscopy for Materials Science, University of Antwerp

Institut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven

Laboratory of Nuclear Chemistry, Université Catholique de Louvain

[China, P. R.]
Department of Chemistry, University of Science and Technology of China

Department of Physical Chemistry, University of Science & Technology of China

Institute of Process Engineering, Chinese Academy of Sciences

Jilin Institute of Plastics Industry

State Key Laboratory of Applied Organic Chemistry, Lanzhou University

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University

[Estonia]
Institute of Chemical Physics and Biophysics

[France]
Centre de Geostatistique, Ecole des Mines de Paris, Fontainebleau

[Germany]
Max-Planck- Institut für Kernphysik

Organic and Macromolecular Chemistry, The University of Ulm

[Italy]
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Istituto per i Materiali Composti e Biomedici – CNR

[Korea, R.]
Organosilicon Chemistry Laboratory, Korea Institute of Science & Technology

[Poland]
Department of Respiratory Research, Medical Research Center, Polish Academy of Sciences

Laboratory of Toxicology and Risk Assessment, Institute of Coal Chemistry, Polish Academy of Sciences

[Russia]
Budker Institute of Nuclear Physics, Novosibirsk

Department of Chemistry, Moscow State University

Joint Institute for Nuclear Research (JINR), Dubna

Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences

[Switzerland]
European Organization for Nuclear Research (CERN)

[UK]
Centre for Analytical Sciences, Department of Chemistry, University of Sheffield

School of Chemistry, University of Southampton

[Ukraine]
Magnet Sensor Laboratory, Lviv

National Science Center, Kharkov Institute of Physics and Technology

[USA]
Center for Environmental and Occupational Risk Analysis and Management, Department of Environmental and Occupational Health, College of Public Health, University of South Florida

Department of Chemical Engineering, University of California at Berkeley

Department of Chemistry and Biochemistry, University of California, Los Angeles

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

Department of Interdisciplinary Oncology, H. Lee Moffitt Cancer Center and Research Institute, University of South Florida

Department of Molecular and Cell Biology, University of California Berkeley

Department of Neurosciences, School of Medicine, University of California San Diego

Department of Physics, University of California

Environmental Energies and Technologies Division, Lawrence Berkeley National Laboratory

Infection Control Department, Florida Hospital

Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University

Material Sciences Division, Lawrence Berkeley National Laboratory

Polymers Division, National Institute of Standards and Technology

Stanford Linear Accelerator Center
ENKHUVSHIN, Dorjpalam
D Eng, Kyoto University
"Photoelectrochemical Properties of TiO₂-Based Thin Film Electrodes Chemically Modified by Homogeneous- and Sectional-Doping Processes"
Supervisor: Prof YOKO, Toshinobu
23 March 2004

HATTORI, Masahiro
D Sc, Kyoto University
"Development of a Similarity Measure for Chemical Compound Structures and Analyses of Metabolic Pathways"
Supervisor: Prof KANEHISA, Minoru
23 March 2004

HAYASHIUDA, Minoru
D Sc, Kyoto University
"Structural and Biological Studies on Lectins from the Roots of Pokeweed (Phytolacca americana)"
Supervisor: Prof OKA, Atsuhiko and Prof HATA, Yasuo
23 March 2004

HORI, Yuichi
D Pharm Sc, Kyoto University
"Design of Artificial Proteins Induced Structural Change by Zinc Ion"
Supervisor: Prof SUGIURA, Yukio
23 March 2004

IKEUCHI, Yoshihiro
D Pharm Sc, Kyoto University
"Synthesis, Antitumor Activity and DNA Interaction of Nitro-5-deazafavin Derivatives as New Bioreductive Drug"
Supervisor: Prof SUGIURA, Yukio
23 March 2004

KITANO, Tatsushi
D Sc, Kyoto University
"Selective Separation of Transition Metal Ions with Tripodal Tridentate Poly(pyrazolyl)borates"
Supervisor: Prof SOHRIN, Yoshiki
23 March 2004

KOMINATO, Kentaro
D Sc, Kyoto University
"Multi-Level Avoided Crossings in High Rydberg States of ⁸⁷Rb"
Supervisor: Prof MATSUKI, Seishi
23 March 2004

MASUNO, Atsunobu
D Sc, Kyoto University
"Control of Physical Properties in Micro-fabricated Perovskite-type Manganese Thin Films"
Supervisor: Assoc Prof TERASHIMA, Takahito
24 November 2004

MIYAKE, Kousuke
D Sc, Kyoto University
"Magnetism and Magnetoresistance of Magnets with Nanocontacts Prepared by Nanofabrication Technique"
Supervisor: Prof MIJU, Ko
23 January 2004

MURAKAMI, Miwa
D Eng, Kyoto University
"Studies on the Structure Formation and Dynamics of Main-Chain Thermotropic Liquid Crystalline Polymers"
Supervisor: Prof HORII, Fumitaka
24 May 2004

SAGAWA, Takashi
D Eng, Osaka City University
"Mechanistic Studies on Catalytic Addition of Inter-element Linkages"
Supervisor: Prof OZAWA, Fumiyuki
25 March 2004

SHIBATA, Masahiro
D Sc, Kyoto University
"Microwave Single-Photon Detection with Rydberg Atoms at Low Temperature"
Supervisor: Prof MATSUKI, Seishi
23 March 2004

TAKAHASHI, Nobuki
D Eng, Kyoto University
"Structure Formation and Microscopic Dynamics of Poly(vinyl alcohol) Gels"
Supervisor: Prof KANAYA, Toshiji
23 March 2004

TAKAEBAYASHI, Yoshihito
D Sc, Kyoto University
"Dipolar Hydration Structure from Ambient to Supercritical Conditions"
Supervisor: Prof NAKAHARA, Masaru
24 May 2004

TAKIYASHI, Masanori
D Med Sc, Kyoto University
"Physiological and Pathological Roles of Septin 3 in Human Barain"
Supervisor: Prof UEDA, Kunihiro
24 May 2004

TAN, Hendra
D Eng, Kyoto University
"Linear and Nonlinear Rheological Properties of Diblock and Triblock Copolymer Systems"
Supervisor: Prof WATANABE, Hiroshi
24 May 2004

TERASAKI, Tadatsumi
D Pharm Sc, Kyoto University
"Creation of New Non-Nucleotide Adenosine Deaminase Inhibitors by Structure-Based Drug Design"
Supervisor: Prof SUGIURA, Yukio
23 March 2004

WEI, Yan-Lin
D Agr, Kyoto University
"Studies of Enzymes from Cold-adapted Microorganisms and Construction of Their Overproduction Systems"
Supervisor: Prof ESAKI, Nobuyoshi
23 March 2004
YAJI, Toyonari
D Sc, Kyoto University
“Study on Phase Transformation Processes in Organic Crystals from Microscopic Observations of Their Surface Morphologies”
Supervisor: Prof. ISODA, Seiji
23 March 2004

YAMAGUCHI, Atsuko
D Inf, Kyoto University
“Algorithms for Graph Theoretic Optimization Problems in Bioinformatics”
Supervisor: Prof. AKUTSU, Tatsuya
24 November 2004

ZHANG, Jian
D Eng, Kyoto University
“Studies on High Luminance Eu^{2+}-doped Thiogallate Phosphors”
Supervisor: Prof. YOKO, Toshinobu
24 November 2004
THE 104TH ICR ANNUAL SYMPOSIUM
(3 December 2004)

ORAL PRESENTATIONS

TANAKA, Seigo (Molecular Clinical Chemistry)
“Molecular Mechanisms of Regulating Life and Death of the Cells”

MAMITSUKA, Hiroshi (Proteome Informatics)
“Mining from Carbohydrate Data”

- The ICR Award for Young Scientist -
TSUJI, Hayato (Organic Main Group Chemistry)
“Conformation Control of Oligosaccharides Based on Bicyclic Structure”

HIRATAKE, Jun (Chemistry of Molecular Biocatalysts)
“Design of Enzyme Inhibitors to Probe Enzyme Structure and Mechanism”

OKAZAKI, Masaki (Organotransition Metal Chemistry)
“Stepwise Bromination of Two Acetylene Molecules on a Tetrairon Core: Formation and Reactivity of Bromoacetylene - and Dibromoacetylene - Coordinated Clusters”

YOSHIDA, Hiroshi (Molecular Aggregation Analysis)
“Deposition of Acrylonitrile Cluster Ions on Solid Substrates”

NEBOTO, Takashi (Electron Microscopy and Crystal Chemistry)
“Crystal Growth and Nano-fabrication at Liquid/solid Interface”

SHIRAI, Toshiyuki (Particle Beam Science)
“Beam Physics in Electron Storage Ring, KSR”

POSTER PRESENTATIONS

- The ICR Award for Students -
SHINOHARA, Akihiro (Organoelement Chemistry)
“Synthesis of Kinetically Stabilized Silasarmatonic Compounds and Their Properties”

- The ICR Award for Students -
SAITO, Shigeki (Chemistry of Molecular Biocatalysts)
“Arabidopsis CYP707A1 Enzyme (+)-Abscisic Acid 8’-Hydroxylation, a Key Enzyme in the Oxidative Catabolism of Abscisic Acid”

— Organoelement Chemistry —

— Structural Organic Chemistry —

OGAWA, Kohei; KITAGAWA, Toshikazu; KOMATSU, Koichi
“Generation and Properties of a Cyclopentadienyl Cation Annulated with Homosamaranate Frameworks”

LEE, Yangsoo; MASAOKA, Naoki; KITAGAWA, Toshikazu; KOMATSU, Koichi
“Alkylfullerenylications: Their Generation, Isolation, and Stability”

ISHIDA, Shintaro; NISHINAGA, Tohru; WEST, Robert; KOMATSU, Koichi
“NMR Observation of 2-Silaimidazolium Cation and Properties of the Related Compounds”

MAEDA, Shuhei; MURATA, Michihisa; MURATA, Yasuhiro; KOMATSU, Koichi
“Encapsulation of Molecular Hydrogen into an Open-Cage Cu Derivative”
— Synthetic Organic Chemistry —

TANIMA, Daisuke
“Temperature Dependent Visual Enantiomeric Recognition by Phenolphthalein Derivatives”

MONGUCHI, Daiki
“Asymmetric Cyclization Based on Dynamic Chirality of Enolates”

— Chemistry of Polymer Materials —

OHKURA, Masahiro
“Material Design Using Fine Particles Coated with High Density Polymer Brushes”

KWAK, Yongwan; GOTO, Atisushi; FUKUDA, Takashi
“Kinetic Studies on Activation Processes in Organocatalyst- and Organocatalyst-Mediated Living Radical Polymerizations”

KOH, Kyoungmoo
“Precision Synthesis and Application of Tadpole-Shaped Polymers with a Fluorine-Carrying Silsesquioxane”

— Chemistry of Polymeric Functionality Materials —

“Recent Studies in the area of Chemistry of Polymeric Functionality Materials”

YOSHIKOA, Tairyo; FUTUMURA, Takashi; TSUJI, Masaki; KOHJII, Shinzo
“Morphological Study on Crystalline Thin Films of PBT”

MATUDA, Shotaro; SENNO, Kazunobu; KOHJII, Shinzo
“Physical Gelation of Syndiotactic Polystyrene in the Presence of Poly(ethylene oxide)”

— Inorganic Photonics Materials —

KUNIYOSHI, Minoru
“Preparation of Organic-Inorganic Hybrid Polysiloxane Low-Melting Glasses with High Ultraviolet Transparency”

IKAWA, Hiroiuki
“Optical Characterization of the Space Charge Layer in Thin Film TiO2 Electrodes”

MASAI, Hirokazu
“Effect of the Organic Groups on the Formation of Siloxane Network through Gel-Melting Method”

HIDAKA, Kenji
“Preparation of Sandwich-type TiOx/AmOx/TiOx (M=V and Cr) Multilayer Thin Film Electrodes Via Sputtering Method”

— Magnetic Materials —

“Spin Induced Transport Phenomena in Nano-scale Ferromagnets”

HIMENO, Atsushi
“Ratchet Effect of a Magnetic Domain Wall in Submicron Magnetic Wires with Asymmetric Periodical Notches”

— Biofunctional Design-Chemistry —

HIRATA, Tsuyoshi
“50 Base Pairs Recognition and Altered DNA Binding Mode by the Longest Artificial 15-Zinc Finger Protein”

MASUI, Yumi
“Improvement of Transfection Efficiency by the Addition of pH-sensitive Peptide”

— Chemistry of Molecular Biocatalysts —

SHIMIZU, Bun-ichi; TAMAI, Michiko; KAI, Kosuke; SAKATA, Kanaro
“Tracer Analysis of the Oxidation Step in Biosynthesis of Coumarins in Sweet Potato Using 18O2”

FUJITA, Satomi; OHNISHI, Toshiyuki; WATANABE, Bunta; MIZUTANI, Masaharu; SAKATA, Kanaro
“Biochemical Analysis of Plant Cytochrome P450 Monoxygenases in Brassinosteroid Biosynthesis”

— Molecular Biology —

OKA, Atsuhiko; AYOAMA, Takashi; YASUDA, Keiko; TANOYU, Masatoshi
“Function and Target Gene Analyses of the Arabidopsis Response Regulator ARR1 Capable of Transactivation”

TSUGE, Toshitaka; OKA, Atsuhiko
“CSN: The Key Complex Linking Environmental Signals to Morphogenesis in Plants”

IMAO, Komiko
“Function Analysis of AtCYCA2;3 in Regulation of Endoreduplication”

— Molecular Clinical Chemistry —

TAKAGI, Junpei; TAKEHASHI, Masanori; TANAKA, Seigo
“Mitochondrial Impairment Induced by Poly(ADP-ribose) polymerase-1 Activation after Cerebral Ischemia”

TAKEHASHI, Masanori; TANAKA, Seigo
“Expression and Complex-formation of Brain-specific Protein Septin 3”

— Molecular Materials Chemistry —

YAMADA, Tomonori; TSUKAMOTO, Naoki; KUSAKA, Yasunari; KAIJI, Hiroshi; HORII, Fumitaka
“Precise Structure Analysis of Organic EL Materials by Solid-State NMR and Quantum Chemical Calculations”

SUZUKI, Fumitosu; TSUJITANI, Koji; HIRAI, Asako; HORII, Fumitaka
“Structure and Structural Change of Sub-elementary Fibers of Bacterial Cellulose in an Initial Period of Layered System Organization”
— Hydrospheric Environment Analytical Chemistry —
| 17 | NORISUE, Kanjirou |
| “Distribution of Trace Metals in the Sulu Sea and Its Adjacent Basins” |

— Solution and Interface Chemistry —
| 17 | OKAMURA, Emiko; WAKAI, Chihiro; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru |
| “Molecular Dynamics in Lipid Membranes and Drug Delivery by NMR” |
| 17 | NAGAI, Yasuharu; MOROOKA, Saiko; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru |
| “Noncatalytic Reactions of Aldehyde and Ether in Supercritical Water” |

— Molecular Microbial Science —
| 17 | KUROKAWA, Suguru |
| “Physiological Function of Selenocysteine Lyase” |
| 17 | KAWAMOTO, Jun |
| “Proteome Analysis of a Psychrotrophic Bacterium, Shewanella sp. Ac10, to Elucidate Its Cold-adaptation Mechanism” |

— Polymer Materials Science —
| 17 | “Accurate Analysis for Higher Order Polymer Structure” |
| 17 | KAWAI, Takahiko; STROBL, Gert; KANAYA, Toshiji |
| “Crystallization of a Poly(ethylene-co-octene): A Precursor Phase and two Competing Mechanisms” |

— Molecular Rheology —
| 17 | “Perspective of Molecular Rheology” |
| 17 | KIKUCHI, Toshimitsu |
| “Electric Birefringence of Amorphous Polymers” |

— Molecular Aggregation Analysis —
| 17 | YAMAGUCHI, Takayuki |
| “Molecular Photoelectron Spectroscopy of BMDCM” |
| 17 | ASAMI, Koji |
| “Dielectric Relaxation in Microemulsions Near Temperature-dependent Phase Inversion” |

— Supramolecular Biology —
| 17 | TAKAHARA, Keigo; TAKEUCHI, Ken-ichi; UMEIDA, Masato |
| “The Role of Fatty Acid Desaturase in Energy Metabolism of Organisms” |
| 17 | TANJUCHI, Kentaro; INADOME, Hironori; KATO, Utao; TAKEUCHI, Ken-ichi; UMEIDA, Masato |
| “Regulation of Cell Morphology and Cell Size in Multicellular Organisms” |

— Particle Beam Science —
| 17 | YAMAZAKI, Atsushi |
| “Generation of a Monoenergetic Electron Beam Using a Single Laser Pulse” |
| 17 | FUJIMOTO, Shinji |
| “Non-destructive Beam Monitor Development for a Small Ion Storage Ring S-LSR” |
| 17 | TAKEUCHI, Takeshi |
| “Magnetic Field Measurement of Quadrupole Magnets and Accelerator Alignment for S-LSR” |
| 17 | TONGU, Hiromu |
| “Improvement of Beam Lifetime in the Electron Storage Ring, KSR” |
| 17 | TANABE, Mikio; SHIRAI, Toshiyuki; IKUGAMI, Mamshi; TONGU, Hiromu; NODA, Akira |
| “Design of the Deflection Elements for Dispersion Control” |

— Laser Matter Interaction Science —
| 17 | SHIMIZU, Seiji |
| “Desorption/Ionization Induced by an Intense Short Pulse Laser” |

— Electron Microscopy and Crystal Chemistry —
| 17 | “Research Topics in Our Laboratory” |

— Organic Main Group Chemistry —
| 17 | MATSUNAGA, Tadafumi |
| “Cross-coupling Reaction of Aryl- and Alkenyl-trifluoromethanes with 1-arylaziridines Using a Palladium Catalyst” |
| 17 | SASI, Shihen |
| “Synthesis of Diallyl-pyridine Oligomers” |

— Advanced Solid State Chemistry —
| 17 | “Transition Metal Oxides - Functions and Synthesis -” |
| 17 | KAN, Daisuke |
| “Fabrication and I-V Characteristics of p-n Junctions Composed of High-Tc Superconductors and La-doped SrTiO3” |
YAMADA, Ikuya
"Synthesis, Structure of Ca$_2$CuOyCl$_2$

— Organotransition Metal Chemistry —

Katayama, Hiroyuki
"(Z)-Selective Cross-dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinyldenerruthenium Complexes"

— Bioknowledge Systems —

"Bioknowledge Database KEGG and Its Application to Bioinformatics"

KOTERA, Masaki
"Development of the EC Number Prediction System Based on Changes of Reactant Structures"

— Biological Information Network —

"Computational Analysis of Structures of Biological Information Networks and Chemical Compounds"

— Bioinformatics Training Unit —

Kato, Kazuaka
"Multiple Sequence Alignment Program MAFFT"
SEMINARS

Prof. ASANO, Tsutomu
Faculty of Science, Shizuoka University, Japan
"Initial Stage of Crystallization of Polymer or Crystallizable Material"
28 June 2004

Prof. BANKAITE, Vyta A.
Department of Cell & Developmental Biology, School of Medicine, University of North Carolina, USA
"Phosphatidylinositol Transfer Proteins: Novel Signaling Functions in Higher Eukaryotic Membrane Trafficking"
26 April 2004

Prof. BEN-NAIM, Arieh
The Hebrew University of Jerusalem, Israel
"Cooperativity in Biochemical Binding Systems"
10 March 2004

Prof. BOPP, Philippe A.
Univ. Bordeaux I, France
"Modeling Time-Resolved Spectroscopies HDOR in D2O or A Very Simple Model of Intermolecular Energy Relaxation in Order to Study Energy Flows in Liquids"
10 June 2004

Prof. CHHIABRA, Raj P.
Indian Institute of Technology, Kanpur, India
"Flow of Power Law Fluids Past a Square Bar"
6 July 2004

Prof. CLAYDEN, Jonathan
Department of, University of Manchester, England
"Controlling the Stereochemistry of Tertiary Amides and Their Lithio Derivatives"
26 March 2004

Prof. DJIBO, Gabor
Institute of Chemistry, Eotvos L. University, Hungary
"A New Approach for High-Throughput Screening"
22 October 2004

Prof. FERRE, Jacques
Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France
"Magnetooptical Study of the Magnetization Reversal Dynamics in Ultrathin Films and Patterned Structures"
13 May 2004

Dr. FLEISCHMANN, Hans-Peter
Institute of Food Chemistry Technical University of Braunschweig, Germany
"Carotenoid Degradation and Flavor in Japanese Green Tea from Shizuoka Area"
12 October 2004

Dr. FOKINE, Michael A.
Toyota Technological Institute, Japan
"Fiber Based Components: Modulators, Filters and Sensors"
10 December 2004

Dr. FRIEDELIN, Rainer
Department of Physics, Linköping University, Linköping, Sweden
"Photoelectron Spectroscopy on Li-Intercalation Compounds of Aromatic Molecules: Can We Optimize the Carbon-Based Electrode in Li-ion Batteries?"
7 September 2004

Prof. FUKUI, Kiyoshi
Institute for Enzyme Research, University of Tokushima, Tokushima, Japan
"Molecular Enzymology of D-Amino Acid Oxidase and a New Apoptosis-Inducing Molecule Nucleating"
9 February 2004

Prof. FURUYA, Hidemine
Tokyo Institute of Technology, Tokyo, Japan
"Correlation between Molecular Dynamics and Local Structure in Amorphous Polymers"
25 October 2004

Prof. GASPAR, Peter P.
Washington University, USA
"Learning from Silylenes and Supersilylene"
4 November 2004

Dr. GRIESSER, Manfred
Max Planck Institute für Kernphysik, Heidelberg, Germany
"The Accelerator Facility at MPI for Nuclear Physics in Heidelberg - TSR, CSR and USR (Contribution to Flair)"
9 November 2004

Prof. HAESENDONCK, Chris Van
Laboratory of Solid-State Physics and Magnetism, Katholieke Universiteit Leuven, Belgium
"Studying Ferromagnetism with Combined Magnetic Force Microscopy and Magnetoresistance Measurements"
21 May 2004

Prof. HAN, Yanchun
Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, China P.R.
"Micro/Nano-Patterning of Thin Polymer Films with Reversibly Switchable Properties"
17 November 2004

Dr. HANAGURI, Tetsuro
Magnetic Materials Laboratory, RIKEN, Wako, Japan
"STM/STS Studies on a Lighly-doped Cuprate Ca0.65CuO2Cl2"
2 November 2004

Prof. HERGES, Rainer
Universität Kiel, Germany
"Approaching the Rational Synthesis of Carbon Nanotubes"
30 September 2004

Prof. HIROI, Zenji
Institute of Solid State Physics, University of Tokyo, Tokyo, Japan
"Chemistry and Physics of Transition Metal Oxides"
17 February 2004

Prof. Eri HORIE, Kazuyuki
The University of Tokyo, Tokyo, Japan

114 SEMINARS
“Microscopic Light Scattering of Polymer Gels and Optical Control of Polymer Gels and Liquid Crystals”
9 December 2004
Prof. HUDECZ, Ferenc
Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary
“Oligo- and Polypeptide Targeting of Drugs, Epitopes and Reporter Molecules”
25 October 2004
Dr. JEONG, Young Uk
Korea Atomic Energy Research Institute, Daejeon, Korea
“Compact Terahertz-range Free-Electron Laser and its Application”
5 January 2004
Prof. KAGAN, Henri Boris
Institut de Chimie Moléculaire et des Matériaux, Université de Paris-Sud, France
“Double Asymmetric Catalytic Reactions, Principle and Application”
19 November 2004
Dr. KIKUTANI, Eiji
High Energy Accelerator Research Organization, Tsukuba, Japan
“Status and Future of KEKB”
2 March 2004
Prof. KISHIO, Koji
Graduate School of Engineering, University of Tokyo, Tokyo, Japan
“Magnetoo-science and Magnetoochemistry”
12 March 2004
Dr. KRAKOVSKY, Ivan
Charles University, Czech Republic
“Structure and Properties of Hydrophilic Epoxy Network”
20 October, 2004
Prof. KUROKAWA, Shin-ichi
High Energy Accelerator Research Organization, Tsukuba, Japan
“Achievement of KEK-B Factory”
29 September 2004
Prof. KUROKAWA, Shin-ichi
High Energy Accelerator Research Organization, Tsukuba, Japan
“Present Situation of Accelerators in Asia”
29 September 2004
Research Planning Director, KYOTO, Michihisa
Sumitomo Electric Industries, Ltd., Osaka, Japan
“Strategy in Research & Development at Sumitomo Electric Industries, Ltd.”
13 December 2004
Dr. LEE, Ki-ae
Korea Atomic Energy Research Institute, Daejeon, Korea
“Generation of Intense Attosecond X-ray Pulse using Relativistic Nonlinear Thomson Scattering”
5 January 2004
Prof. LIN, Yuzheng
Tsinghua University, Beijing, China P. R.
“The Recent R&D of Electron Linacs and Their Applications at Tsinghua University”
18 March 2004
Prof. LIU, Yunqi
Institute of Chemistry, Chinese Academy of Sciences, Beijing, China P. R.
“Organic/polymeric Light-emitting Diodes”
22 January 2004
Prof. LIU, Yunqi
Institute of Chemistry, Chinese Academy of Sciences, Beijing, China P. R.
“Phthalocyanines: Synthesis, Characterization and Their Application in Electronic Devices”
22 January 2004
Senior Researcher MACHIDA, Masayuki
Research Center for Glycoscience, National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan
“From Basic Genetic Engineering to Functional Genomics”
16 January 2004
Senior Researcher MACHIDA, Masayuki
Research Center for Glycoscience, National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan
“What is Functional Genomics?”
20 February 2004
Senior Researcher MACHIDA, Masayuki
Research Center for Glycoscience, National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan
“The Relation between the Progress of Technology and the Evolution of Functional Genomics”
18 March 2004
Dr. MAGONOV, Sergei
Digital Instruments / Veeco Metrology, USA
“Visualization of Polymer Structures with Atomic Force Microscopy: From Individual Macromolecules to Bulk and Multicomponent Materials”
14 June 2004
Dr. MARGETIC, Davor
Rudjer Boskovic Institute, Croatia
“Novel Thermal Isomerizations of Cyclobutane Di(carboxymethoxy)tetraolines Involving Intramolecular 1,3-Dipolar Cycloaddition”
20 January 2004
Prof. MARTIN, Nazario
Complutense University, Spain
“Mimicking Photosynthesis: The Quest for Highly Stabilized Radical-Ion Pairs in Functionalized Fullerenes”
25 June 2004
Prof. MESHKOV, Igor N.
Joint Institute for Nuclear Research (JINR), Dubna, Russia
“Some Peculiarities of Electron Cooling at Low Ion Energy”
19 April 2004
Dr. MICHEL, Sarah, L. J.
Maryland University, USA
“Selective RNA Binding Properties of a Non-Classical Zinc Finger Protein Involved in Inflammatory Response (NUP-475): A Peptide Mimetic Approach”
16 November 2004
Prof. MÜLLER, Axel H. E.
Bayreuth University, Germany
“New Amphiphilic and Hybrid Nanoparticles: Janus Micelles, Core-Shell Cylinders, Nanomagnets, Nanowires”
10 December 2004
CEO and Chairman NAGASAWA, Koichi
Renesas Technology Corporation, Tokyo, Japan
“Current status and Future of the Semiconductor Industry”
13 December 2004
Prof. NELLIS, William J.
Harvard University, USA
“The Semiconductor-Metal Transition in Fluid H, O, N, Rb, and Cs at High Pressures”
13 September 2004
Prof. NG, Michael Kwok-Po
Department of Mathematics, the University of Hong Kong, Hong Kong, China P.R.
“On Discovery of Extremely Low-dimensional Clusters Using Semi-supervised Projected Clustering”
21 October 2004
Prof. NICIULESCU, Peter
Max-Born-Institute, Berlin, Germany
“Interaction of Short Intense Laser Pulses with Matter, -Activities at the Max-Born-Institute Berlin -”
17 June 2004
Dr. PARK, Seong Hee
Korea Atomic Energy Research Institute, Daejeon, Korea
“Preliminary Study of Compton X-ray Source Generation at KAERI”
5 January 2004
Prof. ROSSKY, Peter J.
Institute for Theoretical Chemistry
Department of Chemistry & Biochemistry, University of Texas, USA
“Chemistry in Supercritical Solvents”
9 September 2004
Chief Engineer SATO, Kenichi
Energy and Environmental Technology R&D Laboratories, Sumitomo Electric Industries, Ltd., Osaka, Japan
“Application of Bi-based High-Tc Superconducting Wire”
12 March 2004
Prof. SCHAPER, Andreas
Material Sciences Center, Philipps University in Marburg, Marburg, Germany
“Synthesis, Structure, and Properties of Carbon Nanotubes without and with Metal Filling”
23 February 2004
Prof. SCHAPER, Andreas
Material Sciences Center, Philipps University in Marburg, Marburg, Germany
“Self-organized Modulation and Ordering in Mineral Single Crystals and in Heteroepitaxial Semiconductor Layers”
27 February 2004
Prof. SCHAPER, Andreas
Material Sciences Center, Philipps University in Marburg, Marburg, Germany
“About Spherical and Fibrous Nanomaterials of Different Nature, and for Different Potential Purposes”
12 March 2004
Prof. SCHAPER, Andreas
Material Sciences Center, Philipps University in Marburg, Marburg, Germany
“Electron Microscopic Study of Quasicrystals”
16 March 2004
Prof. SCHMUTZLER, Reinhard
Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Germany
“Oxidative Addition and Insertion Reactions of Hexafluoroacetone and Perfluoroinated 1,2-Diketones to Compounds of Low-valent Phosphorus - New Modes of Addition and Unusual Products”
25 March 2004
Prof. SHEVELKO, Viatcheslav P.
Lebedev Physical Institute Russian Academy of Science Leading Scientist, Moscow, Russia
“Target Density Effects in Collisions of Fast Ions with Solid Targets”
30 November 2004
Dr. SHIMIZU, Hirohiko
RIKEN, Saitama, Japan
“Small-angle Neutron Scattering using Magnetic Focusing Lens”
19 May 2004
Dr. SIDORIN, Anatoly
Joint Institute for Nuclear Research (JINR), Dubna, Russia
“Simulation of Particle Dynamics in Presence of Electron Cooling using BETACOOL Code”
6 February 2004
Dr. SMIRNOV, Alexandre Valentinovich
Joint Institute for Nuclear Research (JINR), Dubna, Russia
“Simulation of Crystalline Beams in Storage Ring using BETACOOL Code”
6 February 2004
Prof. STANGNER, Amnon
Technion (Israel Institute of Technology)
“Another Story of Aromaticity that is Told by Strained Aromatic Compounds”
12 February 2004
Prof. STREUBEI, Rainer
Institut für Anorganische Chemie, Universität Bonn, Germany
“Electrophilic Terminal Phosphinidene Complex-Coordination Chemistry of a Group 15 Element”
6 December 2004
Dr. STROSZNAJDER, Robert
Department of Neurophysiology, Medical Research Center, Polish Academy of Sciences, Warsaw, Poland
“Poly(ADP-ribose) in Neurodegeneration”
1 November 2004
Dr. SUBRAMANIAN, Mas
Experimental Station, DuPont CR&D, Wilmington, USA
“Magnetic Perovskites: Magneto Capacitance, Colossal Dielectrics and Valence Degenerate Metals”
26 October 2004
Prof. SUGAWARA, Tadashi
Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, Japan
“Towards Self-Replicating Systems”
2 July 2004
Prof. SYRESIN, Evgeny
Joint Institute for Nuclear Research (JINR), Dubna, Russia
“Formation of Cooled Ion Beams in Compact Synchrotrons and Storage Rings”
24 February 2004
Prof. TAKAHASHI, Hideaki
Graduate School of Engineering Science, Osaka University, Osaka, Japan
“Fundamentals and Applications of Hybrid First-Principles Molecular Dynamics Simulations”
28-29 January 2004
Prof YOUNG, Petey
Southern Oregon University, USA
“Writing for Publication in English”
16 October 2004

Assoc Prof TAKEDA, Shigenobu
Department of Aquatic Bioscience, University of Tokyo, Tokyo, Japan
“A Variety of Iron-utilization Processes by Marine Phytoplankton”
20 December 2004

Dr TANAKA, Katsu
Chemistry Department, Columbia University, USA
“Configurational Studies of Olefin-Containing Natural Products by Cross Metathesis/CD Analysis”
9 October 2004

Prof TEIXIDOR, Francesc
Consejo Superior de Investigaciones Científicas (C.S.I.C.), Spain
“Relevance of the Electronegativity of Boron in $\delta^-$-Coordinating Ligands. Regioselective Monoalkylation and Monoarylation in Cobaltbis(dicarbollide) [3,3$'$-Co(1,2-C$_4$B$_{11}$H$_{12}$)$_2$]- Clusters”
6 December 2004

Dr TONGE, Matthew P.
UNESCO Center of Macromolecules and Materials, Stellenbosch University, South Africa
“Mechanistic Studies on RAFT Polymerisation”
3 February 2004

Dr TRACZ, Adam
Center of Molecular and Macromolecular Studies, Polish Academy of Sciences, Poland
“Crystallization of Polyethylene at Melt/atomically Flat Solid Interface; AFM studies”
12 March 2004

Senior Research Scientist TSUKAGOSHI, Kazuhito
RIKEN, Japan
“Nano-Science and Nano-Technology”
27-28 September 2004

Dr UTSUMI, Wataru
Synchrotron Radiation Research Center, Japan Atomic Energy Research Institute, Mikazuki, Hyogo, Japan
“Congruent Melting of Gallium Nitride at 6 GPa and Its Application to Single-crystal Growth”
8 April 2004

Prof VIVES, Eric
University of Montpellier II, France
“Cell Penetrating Peptides: From Mystery to Reality”
16 November 2004

Prof WIST, Robert
University of Wisconsin, Madison, USA
“Some Aromatic Silicon and Germanium Compounds”
16 October 2004

Prof WUNDERLICH, J.
Hitachi Cambridge Laboratory, UK
“Optical Spin Detection of Quasi-Two-Dimensional Charge Carriers: Experimental Evidence of the Spin Hall Effect”
18 November 2004

Prof YAN, Chun-hua
College of Chemistry, Peking University, Beijing, China P. R.
“Rare Earth Separation and Functional Materials Chemistry”
12 October 2004
MEETINGS AND SYMPOSIUMS

The 3rd International Symposium of the Kyoto University COE Project “Elements Science”: “Elements Selection Rule and Materials Science” in Commemoration of the Opening of International Research Center for Elements Science

Organized by TAMAQ, Koji and KOMATSU, Koichi
9-10 January 2004 (ICR, Kyoto)

Scientific Sessions

Prof. KAYA, Koji
Institute for Molecular Science
“Photo-Electron Spectroscopy of Solvated Electrons in Nano-scaled Molecular Clusters: From Dipolar Molecules to Aromatic Molecules”

Prof. BERTRAND, Guy
University of California, Riverside, USA
“Stable Single Diradicals and Tetra-radicals Based on Group 13 and 15 Elements”

Prof. ETOURNEAU, Jean
University of Bordeaux, France
“Electron Localization and Unusual Hysteresis in the Magnetic Susceptibility of Cubic Hexahedrite KBc”

Prof. LEO, Karl
Technical University of Dresden, Germany
“Electrically Doped Organic Semiconductors: Basics and Device Applications”

Prof. SAITO, Gunzi
Graduate School of Science, Kyoto University
“Organic Superconductor with Anisotropic Spin-Lattice: Interplay between Spin-Frustration and Superconductivity in x-(ET)2Cu2(CN)3”

Prof. GULDI, Dirk M.
University of Notre Dame, USA
“Novel Multifunctional Nanodevices in Energy Conversion”

Prof. PENG, Shie-Ming
National Taiwan University, Taiwan
“From Metal String Complexes to Metal Wires”

Prof. LIU, Yunqi
Chinese Academy of Sciences, China P. R.
“Electronic Devices Based on Multiwalled Carbon Nanotubes”

Prof. NAKAMURA, Eiichi
The University of Tokyo
“Organic Synthesis: The Gateway to Nanoscience”

Prof. GLEITER, Rolf
University of Heidelberg, Germany
“Weak Forces – Strong Effects. Nanotube Formation Favored by Chalcogen-Chalcogen Interactions”

Prof. TOKITO, Norihiro
Institute for Chemical Research, Kyoto University
“The Latest Frontiers of Organoelement Chemistry”

Prof. MANNERS, Ian
The University of Toronto, Canada
“Functional and Supramolecular Metallopolymers”

Prof. OSUKA, Atsuhiro
Graduate School of Science, Kyoto University
“Exploration of Novel Porphyrins; Meso-meso Coupled Porphyrin Arrays and Expanded Porphyrines”

Prof. SCHLOSSER, Manfred
Swiss Federal Institute of Technology, Switzerland
“The 2 x 3 Toolbox of Organometallic Methods for The Regiochemically Exhaustive Functionalization of Aromatic and Heterocyclic Substrates”

Prof. SUGIURA, Yukio
Institute for Chemical Research, Kyoto University
“Potential of Arginine-Rich Peptides as Carriers for Intracellular Protein Delivery”

Prof. TATSUMI, Kazuyuki
Nagoya University
“Transition Metal Sulfides -Synthetic Models of the Nitrogenase Active Sites”

Poster Sessions

Kousaku Miyake and Ko Miibu
“Magnetism and Magnetoresistance Effect of NiFe Wires or Dots with Nanocontacts”

Takuya Okuno and Ko Miibu
“Temperature Dependence of Switching Field of Turned-up Magnetization in CoNbZr Circular Dots”

Takuo Okochi, Ko Miibu, Nobuyoshi Hosoiyo, and Hiroo Hashizume
“Induced Spin Polarization in Non-magnetic Layers of Magnetic/Non-magnetic Metallic Multilayers”

Norihiro Jiko and Ko Miibu
“Magnetism of Cr-based Multilayers”

Shinpei Yamamoto and Mikio Takano
“Nanocomposite Magnet Prepared by Core-Shell Nanoparticle”

Shintaro Ishiwata, Masaki Azuma, and Mikio Takano
“Pressure-induced Insulator to Metal Transition in Bi(BO3)2”

Seiji Niitaka, Masaki Azuma, Mikio Takano, Eiji Nishibori, Masaki Takata, and Makoto Sakata
“High-pressure Synthesis and Physical Properties of Bi-containing Transition Metal Oxides BiCrO3 and BiCoO3”

Dan Wang, Ranbo Yu, Masaki Azuma, Takahito Terahishima, and Mikio Takano
“Solvo-Thermal Synthesis of Novel Low-Dimensional Zirconium Phosphates”

Daisuke Kan, Takahito Terahishima, Mikio Takano, and Akio Yamakawa
“Preparation and Optical Properties of Single-Crystalline CuCu2O Thin Film with Infinite Layer Structure”
Atsushi Ishizumi, Hiroki Matsubara, and Yoshihiko Kanemitsu
“Optical Properties of Semiconductor Nanocrystals Doped with Luminescence Centers”

Hideyuki Inoue, Yoshihiko Kanemitsu, Takami Shimizu, and Mikio Miyake
“Femtosecond Optical Responses in a Self-organized Metal Nanoparticle System”

Takehiko Nagai, Hideyuki Inoue, and Yoshihiko Kanemitsu
“Luminescence Properties of Highly Excited GaN Films”

Megumi Mizuno, Masahide Takahashi, Yonei Tokuda, and Toshimobu Yoko
“Formation of Organic-inorganic Hybrid Low-melting Glasses Via Acid-base Reaction of Phosphoric Acid and Chlorosilane”

Masanori Saito, Hiroshi Kikuchida, Yonei Tokuda, Masahide Takahashi, and Toshimobu Yoko
“Laser Fabrication of Organic-inorganic Hybrid Low-melting Glass Prepared through Non-aqueous Acid-base Reaction”

Yonei Tokuda, Masahide Takahashi, and Toshimobu Yoko
“Inhomogeneous Distribution of Local Structures around Na Ion in Silicate Glasses by 29Na MQMAS NMR Spectroscopy”

Masahide Takahashi, Yonei Tokuda, and Toshimobu Yoko
“Photochemical Reactions Responsible for Photorefractive Index Change in Germanosilicate Glasses”

Hirokazu Masai, Masahide Takahashi, Yonei Tokuda, and Toshimobu Yoko
“Effect of the Organic Groups on the Formation of Siloxane Network”

Deepakam Enishatuvish, Masahide Takahashi, and Toshimobu Yoko
“Effects of the Accumulated VO2-rich Regions on the Photoelectrochemical Performance of the Sol-gel Derived Ti3+xV4-xO7: Thin Film Electrodes”

Yoichihiro Harada, Naoki Sato, Takahito Terashima, Ryoko Kanda, and Mikio Takano
“A study of Oxide Thin Films towards Transparent Electrode Materials”

Hiroyuki Yoshida and Naoki Sato
“Characterization of a Thin Film Prepared by the Deposition of Cluster Ions of Acrylonitrile on a Substrate”

Jun-ya Tsutsumi, Hiroyuki Yoshida, Naoki Sato, Inta Muzikante, and Ojars Neiandis

Kazukuni Nishimura, Guzni Saito, Chien Hong Chong, Masaru Mackhe, Salavat Khasanov, Hideki Yamochi, Akihito Otsuka, Kenji Kanada, Koji Otaka, and Jun Kawamata
“The Estimation of Intramolecular Ionicity, Dipole Moments and (Hyper)polarizabilities in the D∞n-A∞n Zwitterions Prepared from Indoline and TCNQ Derivatives”

Hideki Yamochi, Akira Ota, and Guzni Saito
“Status of (EDO-TTF)_2PF6 at Present”

Masasumi Sakata, Mitsuhiko Maesato, Akira Ota, Hideki Yamochi, and Gunzi Saito
“The Uniaxial Strain Effect on Transport Property of (EDO-TTF)_2PF6”

Yukihiro Yoshida, Mitsuhiko Maesato, Hideki Yamochi, and Gunzi Saito
“Triangular Spin Lattice Based on Low-Symmetrical EOET-TTF”

Mitsuhiko Maesato, Yasuhiro Shimizu, Gunzi Saito, Kazuaya Miyagawa, and Kazuhiro Kanoda
“Role of Anisotropy in the $\gamma$-type Structure of the BEDT-TTF Salts”

Masaya Soeda, Jun Hagiwara, Hideki Yamochi, and Gunzi Saito
“Synthesis of New Donor Molecule, TP-EDOT and Preparation of its PF6 Complex”

Tsunoshi Haneda, Hideki Yamochi, Gunzi Saito, Adam Tracz, Jacek Ulanski, Olga Drozdova, and Kyuya Yakuishi
“Humidity Sensitive Conductivity of (BEDO-TTF)Br(CH3) as a Bulk Property”

Junichi Fuji, Yukihiro Yoshida, Koji Marui, Akihito Otsuka, and Gunzi Saito
“1-Ethyl-3-methylimidazolium Based Ionic Liquids Containing Cyano Groups: Synthesis, Physical Property and Crystal Structure”

Yoshikazu Unemoto, Yasushi Morita, Eigo Miyazaki, Suguru Mak, and Kazuhiro Nakasugi
“Syntheses and Physical Properties of an Ethyleneedithio-TTF Derivative with Butylcarbazol and Its CT Complexes”

Takeshi Ishiiya, Shogo Yamamoto, and Fumiuki Ozawa
“Synthesis and Reactions of Hydridoplatinum(II) Complexes Bearing Diphosphanediocyclobutene (DPCB) Ligands”

Takashi Sagawa and Fumiuki Ozawa
“Alkyno-Insertion into Group 14 Element Platinum Bonds”

Hiroyuki Katayama, Yosuke Fukuk, Masato Nagao, and Fumiuki Ozawa
“Highly Selective Ring-Opening Cross-Metathesis Reactions Using Fischer-type Carbene Ruthenium Catalysts”

Masaki Shimizu, Xinyu Liu, and Tamejiro Hiymaya
“A Facile Stereocontrolled Approach to CF3-Substituted Triaryl-ethenes”

Masaki Shimizu, Masanori Katao, Kotaro Watanabe, and Tamejiro Hiymaya
“Novel Liquid Crystalline Compounds Based on 1-Aryl-2,3,5,6,7,8-hexafluorocyclohexa[2.2.2]octane”

Yoshiaki Nakao, Jun Sato, Eiji Shirakawa, and Tamejiro Hiymaya
“ Palladium-Catalyzed Decarboxylative Carbostannylation of Propargyl Esters”

Yoshiaki Nakao, Shinjiro Ishihara, Yasuhiro Hira, Shinichi Oda, Yuki Honda, Eiji Shirakawa, and Tamejiro Hiymaya
“ Palladium Luminophosphate-Catalyzed Stannylation Cyclization of Conjugated Enynes with Dicyne”

Masaki Shimizu, Takuya Kurashita, Hirota Kitagawa, Katsuhiro Shimono, and Tamejiro Hiymaya
“gem-Silylbrolation Approach to Tri- and Tetrametalmetalanes: the First Synthesis of Boryl(germyl)silyl[stanny]methane”

Hideki Araki, Takeshi Kobayashi, Yutaka Ichihara, Takashi Nakagawa, and Kenji Uneyama
“Mg-Promoted Double Silylation of Trifluoroacetimidoyl Chlorides: A New Entry to the Fluorinated Dianion Equivalents”
Shiroh Futaki, Ikuhiko Nakase, Miki Niwa, Tomoki Suzuki, Daisuke Nameki, Ei-ichi Kodama, Masao Matsuoka, and Yukio Sugiyura
"Intercellular Delivery of RNase S Complex Bearing Arginine-rich Peptides"

Wataru Nomura and Yukio Sugiyura
"Effects of Length and Position of Extended-Linker on Sequence-Selective DNA Recognition of Zinc Finger Peptides"

Michihisa Murata, Yasujiro Murata, and Koichi Komatsu
"Synthesis of Open-Cage Fullerene Derivatives and 100% Encapsulation of a Hydrogen Molecule"

Tetsuya Yamazaki, Aihong Han, Jing-Rong Lin, Yasujiro Murata, and Koichi Komatsu
"Synthesis and Polymerization of the Propylenedioxy-Substituted Thiepophene- Fullerene Dyad"

Yangsoo Lee, Toshikazu Kitagawa, and Koichi Komatsu
"Charge-Transfer-Promoted Substitution of Alkyl C60 Chloride by Proton pongo"

Takayuki Uta, Tohru Nishinaga, and Koichi Komatsu
"Reactions of Benzene and COT Fully Annulated with Bicyclo[2.1.1]hexane"

Rika Nagita, Tohru Nishinaga, Daisuke Yamazaki, and Koichi Komatsu
"Synthesis and Properties of Bis[bicyclo[2.2.2]octato]TTF"

Kohsei Ogawa, Toshikazu Kitagawa, and Koichi Komatsu
"Isolation and Structure of Stable Cyclopentadienyl Radical Annulated with Homoadamantene"

"Studies on the Thermochromism of the 1,3-Diazenaphthalenyl Radical in Solution and Solid States"

Noriyoshi Nagahara, Takahiro Sasamori, Nobuhiro Takeda, and Norihito Tokitoh
"Synthesis, Structure, and Properties of a Novel Ferrocenyl-substituted Diphenane Having a Bulky Substituent"

Takahiro Sasamori, Eiko Mieda, Nobuhiro Takeda, and Norihiro Tokitoh
"Studies on Reactivities of Doubly Bonded Systems between Heavier Group 15 Elements toward Elemental Chalcogens"

Nobuhiro Takeda, Hirofumi Hamaki, and Norihito Tokitoh
"Synthesis and Properties of the First Monomeric, Donor-free Lithium β-Diketiminate Stabilized by Bulky Substituents"

Yutaka Ishida and Akira Sekiguchi
"Synthesis, Structure, and Reaction of First Germanium Bishomoaromatic Cation"

Atsushi Wakamiya, Toshihisa Ide, and Shigeo Hamaguchi
"Synthesis and Properties of Triarylorbrazines"

Caihong Xu, Atsushi Wakamiya, and Shigeo Hamaguchi
"Benz[6]octole as a New Building Unit for Fluorescent π-Conjugated Systems"

Shigeo Hamaguchi, Masatake Miyasato, and Kohei Tamao
"Reductive Bergman-Type Cyclization of Cyclic 1,2-Bis[(styryl)eny]benzenes"

Tomoyuki Saeki, Eun-Cheol Son, Tadao Matsuoka, and Kohei Tamao
"Palladium Catalyzed, Lewis Acid Induced Cross-Coupling Reaction of 1- Aryltriarenes with Arenethoronic Acids and Aryl trifluorosilanes"

Hayato Tsuji, Deborghi L. Casher, Martins Katkevicis, Marub Kubota, Tsunetoshi Kobayashi, Akio Toshimitsu, Josef Michl, and Kohei Tamao
"Relationship between Structure and Photophysical Properties of Peralkylated Dsilanes"

Hayato Tsuji, Motoki Togano, Takeshi Katoaka, Yukio Shibano, and Kohei Tamao
"Synthesis and Properties of Porphyrin-Oligosilane-Fullerene Hybrid Molecules"

21st Century COE on Kyoto University Alliance for Chemistry “Organoelement Chemistry Seminar”

Organized by TOKIOT, Norhiro, TAKEDA, Nobuhiro, TAMAO, Kohei; TSUII, Hayato
19 January 2004 (Kyoto, Japan)

UK-JPN Polymer Workshop 2004

Organized by GABRYS, Barbara; KANAYA, Toshiji
1-2 April 2004 (Kyoto, Japan)

Oral Presentations
Prof Em KAJI, Keisuke
Kyoto University
“A Memory of UK-Japan Collaboration”

Prof BUCKNALL, David
University of Oxford, UK
“The Early Stages of Small Molecule Diffusion into Polymer Thin Films”

Prof MATSUSHITA, Yusha
Nagoya University
“Microdomain Structures of Block Copolymers with Wide Composition Distribution”

Prof TSUJI, Yoshio
Kyoto University
“Structure and Properties of High-Density Polymer Brushes”

Dr DALGLIESH, Robert M
Rutherford Appleton Laboratory, UK
“Time Resolved Neutron Reflection from Electrochemical Systems”

Prof KANAYA, Toshiji
Kyoto University
“Glassy Dynamics of Polymer Thin Films”

Prof MUTHUKUMAR, Murugappan
University of Massachusetts, USA
“Polyelectrolyte Physics”

Prof NISHIDA, Koji
Kyoto University
“Structure Formation Due to Repulsive and Attractive Interactions”
Prof. GABrys, Barbara
University of Oxford, UK
Ionomers and Polyelectrolytes: Differences and Similarities

Prof. SHIBAYAMA, Mitsuhiko
University of Tokyo
"Small-angle Neutron Scattering Study of Pressure and Temperature-sensitive Polyelectrolyte Gels"

Prof. GRIFFITHS, Peter
Cardiff University, UK
"SANS Studies of the Interactions between Ionomeric Polymers and Ionic-nonionic Surfactants"

Prof. URAKAWA, Hiroshi
Kyoto Institute of Technology
"Gel Structure and Gelation of Sulfated Polysaccharide"

Dr. McGREEVY, Robert
Rutherford Appleton Laboratory, UK
"Combining Experiment and Modelling for Polymer Systems"

Poster Presentations

Nambo T, Yamauchi Y, Kusuhiro T, Sakuragi S
Kyoto Institute of Technology, JPN
"Micro-convection, Dissipative Structure and Pattern Formation in Polymer Blend Solutions under Temperature Gradients"

Hayashi K, Kizaki S, Sakuragi S, Iijima Y"1, Shimizu T"1, Hara S"2, Yamamoto K"2, Nakatani S"2
Kyoto Institute of Technology, JPN, KANEKA Corporation, JPN"2, Nagoya Institute of Technology, JPN"2
"Simultaneous SAXS/WAXS/He-SALS Measurements on Crystallization and Spherulite Formation in Phase-Separated Polymer Blends using Synchrotron Radiations"

Takahashi N, Kanaya T, Nishida K, Kaji K
Kyoto University, JPN
"Neutron Spin-Echo Studies on Three Types of Poly(vinyl alcohol) Gels"

Miyazaki T"1, Nishida K"2, Kanaya T"2
Nitto Denko Corporation, JPN"2, Kyoto University, JPN"2
"Thermal Expansion Behavior of Thin Polymer Films"

Takehata H, Takenaka K, Shiomi T
Nagasaki University of Technology, JPN
"Structure Formation in Crystallization of Block Copolymers"

Kimura K, Tsuchida A, Okubo T
Gifu University
"Drying Dissipative Structure of Polymer Solution and Colloidal Dispersion"

Inoue R, Yamano K, Nishida K, Kanaya T, Tsukushi I"1, Shibata K"2, Taylor J. W."1, Levett S. J."1
Kyoto University, JPN, Chiba Institute of Technology, JPN"1, JAERI, JPN"1, Rutherford Appleton Laboratory, UK"1
"Inelastic Neutron Scattering from Polyethylene Thin Films"

Matsuda G, Ogino Y, Sakamoto S, Kanaya T, Nishida K
Kyoto University, JPN
"Spin-echo Structure in the Drawing Polyethylene Blends with Ultra-high Molecular Weight Component"

Yamauchi Y, Kizaki S, Yokotani K, Sakuragi S
Kyoto Institute of Technology, JPN
"Effect of the Sample Thickness on Oscillating Microscopic Convection in a Thin Layer of a Polymer Solution under a Temperature Gradient"

Konishi T, Nishida K, Matsuda G, Kanaya T
Kyoto University, JPN
"Crystallization and Mesomorphic Phase Formation of Isotatic Polypropylene"

Ogino Y, Makusha G, Sharma L, Nishida K, Kanaya T
Kyoto University, JPN
"Crystallization of Isotatic Polypropylene under Shear Flow"

Akemura M, Murakata S, Sakuragi S
Kyoto Institute of Technology, JPN
"Effects of the Pressure on Regularity of Cylindrical Microdomains in Block Copolymers"

Senou K, Atsumi K, Kohjiya S, Ikeda Y"1
Kyoto University, JPN, Kyoto Institute of Technology, JPN"1
"Increase of the Ion Conductivity with the Uniaxial Stretching of High Molecular Weight Poly(ethylene oxide)"

Sharma L, Ogino Y, Nishida K, Kanaya T, Sakamoto S, Konishi K, Matsuda G
Kyoto University, JPN
"Bacterial PHB under Shear, Manipulating the Course of Nature?"

Sharma L, Ogino Y, Nishida K, Kanaya T, Doi Y, Iwata T
Kyoto University, JPN, RIKEN, JPN
"Ultra High Molecular Weight PHB and Medium Molecular Weight PHB Blends under Shear; A method for Fibre Formation?"

Kizaki S, Yamauchi Y, Yokotani K, Sakuragi S
Kyoto Institute of Technology, JPN
"Evaluation of the Extent of the Soret Effect in a PS/DOP Solution under a Temperature Gradient by Laser Beam Deflection Method"

Kitamura M, Kakinoki S"1, Hirano Y"2, Oka M"2
Nara National College of Technology, JPN, Osaka Prefecture University, JPN"2, Osaka Institute of Technology, JPN"2
"Molecular Design of Thermoresponsive Polypeptides"

Hirano Y, Okada M, Iuchi T, Kakinoki S"2, Oka M"2
Osaka Institute of Technology, JPN, Osaka Prefecture University, JPN"2
"Synthesis and Conformational Analysis of Poly(diisopropylamide)"

Kakinoki S, Tenaka M, Onoda Y, Oka M, Hirano Y"2
Osaka Prefecture University, JPN, Osaka Institute of Technology, JPN"2
"Synthesis and Conformational Analysis of Poly(triisopropylamide)"

Kakinoki S, Yuge M, Arimoto M, Tenaka M, Oka M, Hirano Y"2
Osaka Prefecture University, JPN, Osaka Institute of Technology, JPN"2
"Synthesis and Conformational Analysis of Poly(tetrapropylamide)"

Kawaguchi T, Nozaki Y, Kaneko F
Osaka University, JPN
"Structure Research of Dialkyl-1,18-octadecanediocetate"

Shirouchi K, Munakata S, Sakurai S, Kurumura H, Suzuki S"2
Kyoto Institute of Technology, JPN, Denki Kagaku Kogyo, K.K."2
"Features of Microphase-separated Structures in SBS/Triblock Copolymers with Different Lengths of End-block Chains"

Funai E, Sakurai S, Okamoto S"2, Yamato M"2, Kimura T"2
Kyoto Institute of Technology, JPN, Nagoya Institute of Technology, JPN"2, Tokyo Metropolitan University"2
"Effects of the Magnetic Field on Cylindrical Microdomain Structures in Polystyrene-block-poly(ethylene-co-but-1-ene)-block-polystyrene Triblock Copolymers"
Sugimoto T, Ji W, Kasazaki T
Nitta Co. Ltd., JPN
"Structure Control of Thermoplastic Polyurethane by Thermal Treatment"

Yamamoto S, Tsuji Y, Fukuda T, Torikai N1, Takeda M,2
Kyoto University, JPN, High Energy Accelerator Research Organization, JPN1, JAERI, JPN2
"The Structure of High-Density Polymer Brushes in a Chemically Identical Polymer Matrix Studied by Neutron Reflectometry"

Torikai N
High Energy Accelerator Research Organization, JPN
"Structural Analysis of Block Copolymer Thin Films by Neutron Reflectivity Measurement"

Koh K, Sugiyama S, Ohto K, Tsuji Y, Fukuda T, Yamashiro M,1
Ootake N, Watanabe K1
Kyoto University, JPN, Chisso Petrochemical Co., JPN1
"Synthesis of Tadpole-Shaped Polymers with Polyhedral Oligomeric Silsesquioxane"

Yoshikawa C, Goto A, Tsuji Y, Fukuda T, Yamamoto K,1
Kishida A1
Kyoto University, JPN, National Cardiovascular Center Research Institute, JPN1
"Precise Surface Design with High-Density Polymer Brushes: Application to a Polymeric Film"

Ogawa H1,2, Noritake T, Tran-Cong-Miyata Q
Kyoto University, JPN1, Kyoto Institute of Technology, JPN2
"Anisotropic Spinodal Decomposition of Polymer Blends Induced by Spatial Confinement"

38th Meeting on Basic Science Division of the Ceramic Society of Japan

Organized by YOKO, Toshinobu
9 July 2004 (Kyoto, Japan)
Index
<table>
<thead>
<tr>
<th>Name Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>[A]</td>
</tr>
<tr>
<td>ABE, Katsumasa 34</td>
</tr>
<tr>
<td>AKAI, Wataru 36</td>
</tr>
<tr>
<td>AKUTSU, Tatsuya 62</td>
</tr>
<tr>
<td>AOKI, Kiyoko F. 64</td>
</tr>
<tr>
<td>AOKI, Norizu 22</td>
</tr>
<tr>
<td>AOYAMA, Takaaki 24</td>
</tr>
<tr>
<td>ARAFAT, Zaima 54</td>
</tr>
<tr>
<td>ARAKAWA, Naofumi 40</td>
</tr>
<tr>
<td>ASAMI, Koji 40</td>
</tr>
<tr>
<td>ASANO, Kimihira 56</td>
</tr>
<tr>
<td>AZUMA, Masaki 10</td>
</tr>
<tr>
<td>[B]</td>
</tr>
<tr>
<td>BELIK, Alexei A. 10</td>
</tr>
<tr>
<td>BROWN, John 62</td>
</tr>
<tr>
<td>[C]</td>
</tr>
<tr>
<td>CHO, Jeong-Yong 22</td>
</tr>
<tr>
<td>[D]</td>
</tr>
<tr>
<td>DAIYASU, Hiromi 66</td>
</tr>
<tr>
<td>[E]</td>
</tr>
<tr>
<td>EBATA, Ichiro 34</td>
</tr>
<tr>
<td>EMOTO, Kazuo 71</td>
</tr>
<tr>
<td>ESAKI, Nobuyoshi 34</td>
</tr>
<tr>
<td>[F]</td>
</tr>
<tr>
<td>FADIL, Hicham 44</td>
</tr>
<tr>
<td>FUJIIHARA, Fuyuki 22</td>
</tr>
<tr>
<td>FUJI, Masao 16</td>
</tr>
<tr>
<td>FUJII, Tomomi 50</td>
</tr>
<tr>
<td>FUJIMOTO, Shintaro 44</td>
</tr>
<tr>
<td>FUJIMURA, Takaaki 14</td>
</tr>
<tr>
<td>FUJITA, Masashi 60</td>
</tr>
<tr>
<td>FUJITA, Satomi 22</td>
</tr>
<tr>
<td>FUKAGAWA, Daiji 52</td>
</tr>
<tr>
<td>FUKAZAWA, Aiko 52</td>
</tr>
<tr>
<td>FUKUDA, Masaki 16</td>
</tr>
<tr>
<td>FUKUDA, Masahiro 16</td>
</tr>
<tr>
<td>FURUTANI, Masahiro 14</td>
</tr>
<tr>
<td>FUTAKI, Shiroh 20</td>
</tr>
<tr>
<td>[G]</td>
</tr>
<tr>
<td>GAO, Yunyan 6</td>
</tr>
<tr>
<td>GIORDANI, Cristian 32</td>
</tr>
<tr>
<td>GOTO, Atsushi 12</td>
</tr>
<tr>
<td>GOTO, Susumu 60</td>
</tr>
<tr>
<td>[H]</td>
</tr>
<tr>
<td>HAMAKI, Hirofumi 4</td>
</tr>
<tr>
<td>HAMASAKI, Maho 42</td>
</tr>
<tr>
<td>HAN, Liyou 22</td>
</tr>
<tr>
<td>HARUTA, Mitsutaka 48</td>
</tr>
<tr>
<td>HASHIDA, Masaki 46,79</td>
</tr>
<tr>
<td>HASHIMOTO, Kousuke 60</td>
</tr>
<tr>
<td>HATA, Chikako 34</td>
</tr>
<tr>
<td>HATA, Yuso 50</td>
</tr>
<tr>
<td>HATTORI, Masahiro 60</td>
</tr>
<tr>
<td>HAYAMI, Arata 54</td>
</tr>
<tr>
<td>HAYASHI, Akito 56</td>
</tr>
<tr>
<td>HAYASHI, Miwa 34</td>
</tr>
<tr>
<td>HAYASHIDA, Morihito 62</td>
</tr>
<tr>
<td>HIDAKA, Kenji 16</td>
</tr>
<tr>
<td>HIGASHI, Chika 20</td>
</tr>
<tr>
<td>HIGASHINO, Kiyotake 8</td>
</tr>
<tr>
<td>HIMENO, Atsushi 18</td>
</tr>
<tr>
<td>HIROI, Asaka 28</td>
</tr>
<tr>
<td>HIRAKAWA, Mika 60</td>
</tr>
<tr>
<td>HIRAMATSU, Takaaki 40</td>
</tr>
<tr>
<td>HIRANO, Yoshiko 4</td>
</tr>
<tr>
<td>HIRATA, Tatsuo 20</td>
</tr>
<tr>
<td>HIRATAKE, Jun 22</td>
</tr>
<tr>
<td>HIZUKURI, Yoshiechi 60</td>
</tr>
<tr>
<td>HONDA, Wataru 60</td>
</tr>
<tr>
<td>HORIGUCHI, Daisuke 50</td>
</tr>
<tr>
<td>HOSHI, Tatsuko 28</td>
</tr>
<tr>
<td>HOSHINO, Wataru 4</td>
</tr>
<tr>
<td>HOSHIYAMA, Daisuke 66</td>
</tr>
<tr>
<td>[I]</td>
</tr>
<tr>
<td>ICHIHARA, Hisako 66</td>
</tr>
<tr>
<td>IGARASHI, Motoki 34</td>
</tr>
<tr>
<td>IGARASHI, Yoshinobu 60</td>
</tr>
<tr>
<td>IKAWA, Hiroki 15</td>
</tr>
<tr>
<td>IKEDA, Yasunori 10</td>
</tr>
<tr>
<td>IKEMATSU, Atsushi 44</td>
</tr>
<tr>
<td>IKUNO, Masaya 28</td>
</tr>
<tr>
<td>IMAI, Kumi 24</td>
</tr>
<tr>
<td>IMANISHI, Miki 20</td>
</tr>
<tr>
<td>INADOME, Hiromi 42</td>
</tr>
<tr>
<td>INOMOTO, Yutaka 34</td>
</tr>
<tr>
<td>INOUE, Rintaro 36,81</td>
</tr>
<tr>
<td>INOUE, Tadashi 38</td>
</tr>
<tr>
<td>INOUE, Tomoyuki 52</td>
</tr>
<tr>
<td>INOUEYU, Hideyuki 58,79</td>
</tr>
<tr>
<td>INUKAI, Shinichiro 12</td>
</tr>
<tr>
<td>ISHIKI, Toru 36</td>
</tr>
<tr>
<td>ISHIDA, Shintaro 6,78</td>
</tr>
<tr>
<td>ISODA, Seiji 48</td>
</tr>
<tr>
<td>ITAGI, Masakazu 20</td>
</tr>
<tr>
<td>ITO, Kousuke 34</td>
</tr>
<tr>
<td>ITO, Yoshikazu 50</td>
</tr>
<tr>
<td>ITO, Hiroki 44</td>
</tr>
<tr>
<td>ITOH, Masami 60</td>
</tr>
<tr>
<td>IWAMOTO, Mitsumasa 40</td>
</tr>
<tr>
<td>IWASHITA, Yoshisato 44</td>
</tr>
<tr>
<td>[J]</td>
</tr>
<tr>
<td>JAUREGUI, Ruy 60</td>
</tr>
<tr>
<td>JIAO, Chungheng 8</td>
</tr>
<tr>
<td>JIKO, Norihiko 18</td>
</tr>
<tr>
<td>JITSUMORI, Keiji 34</td>
</tr>
<tr>
<td>[K]</td>
</tr>
<tr>
<td>K. C., Durka Bahadur 62</td>
</tr>
<tr>
<td>KAGAWA, Takeshi 46</td>
</tr>
<tr>
<td>KAI, Kousuke 22</td>
</tr>
<tr>
<td>KAIJ, Hiroshi 28</td>
</tr>
<tr>
<td>KAJIWARA, Takeshi 4,77</td>
</tr>
<tr>
<td>KAKUCHIDA, Hiroshi 16</td>
</tr>
<tr>
<td>KAN, Daisuke 54</td>
</tr>
<tr>
<td>KANAYA, Toshiki 36</td>
</tr>
<tr>
<td>KANDA, Hironori 10</td>
</tr>
<tr>
<td>KANDA, Ryoko 54</td>
</tr>
<tr>
<td>KANDA, Yasuhiro 52</td>
</tr>
<tr>
<td>KANEHISA, Minoru 60</td>
</tr>
<tr>
<td>KANEHISI, Yoshitake 58,79</td>
</tr>
<tr>
<td>KANG, Ken-Seok 16</td>
</tr>
<tr>
<td>KANNAN, Haruhisa 14</td>
</tr>
<tr>
<td>KARLSSON-WHEELLOCK, Åsa 60</td>
</tr>
<tr>
<td>KASAI, Shinya 18</td>
</tr>
<tr>
<td>KATAYAMA, Hiroaki 56</td>
</tr>
<tr>
<td>KATO, Hiroaki 22</td>
</tr>
<tr>
<td>KATO, Masahiro 22</td>
</tr>
<tr>
<td>KATO, Takuto 42</td>
</tr>
<tr>
<td>KATOH, Kazutaka 66</td>
</tr>
<tr>
<td>KAWABATA, Noriko 20</td>
</tr>
<tr>
<td>KAWABATA, Takeo 8</td>
</tr>
<tr>
<td>KAWAI, Masahiro 4</td>
</tr>
<tr>
<td>KAWAI, Takahiko 36</td>
</tr>
<tr>
<td>KAWAI, Yasushi 4</td>
</tr>
<tr>
<td>KAWAKAMI, Daisuke 14</td>
</tr>
<tr>
<td>KAWAKAMI, Shimpai 8</td>
</tr>
<tr>
<td>KAWAMOTO, Jun 34</td>
</tr>
<tr>
<td>KAWANISHI, Yutaka 52</td>
</tr>
<tr>
<td>KAWANO, Shino 60</td>
</tr>
<tr>
<td>KAZUOKA, Takeyuki 34</td>
</tr>
<tr>
<td>KIKUCHI, Toshimatsu 38</td>
</tr>
<tr>
<td>KIMURA, Tomohiro 32</td>
</tr>
<tr>
<td>KINOSHITA, Tomomi 22</td>
</tr>
<tr>
<td>KINUGASA, Masatosh 30</td>
</tr>
<tr>
<td>KITA, Yatsu 40</td>
</tr>
<tr>
<td>KITAGAWA, Yoshikazu 6</td>
</tr>
<tr>
<td>KITAKIMA, Takeki 26</td>
</tr>
<tr>
<td>KITAYAMA, Kaori 34</td>
</tr>
<tr>
<td>KITAZAWA, Koichi 70</td>
</tr>
<tr>
<td>KIWADA, Tatsuo 20</td>
</tr>
<tr>
<td>KIYOMURA, Izumotake 48</td>
</tr>
<tr>
<td>KOHAYASHI, Megumi 4</td>
</tr>
<tr>
<td>KOI, Kyoumoo 12</td>
</tr>
<tr>
<td>KOHIYA, Shino 14</td>
</tr>
<tr>
<td>KOIKE, Yukihito 20</td>
</tr>
<tr>
<td>KOMATSU, Koichi 5</td>
</tr>
<tr>
<td>KOMATSU, Shigeo 52</td>
</tr>
<tr>
<td>KONISHI, Takeki 36</td>
</tr>
<tr>
<td>KOSHINO, Mano 48</td>
</tr>
<tr>
<td>KOTERA, Masaki 60</td>
</tr>
<tr>
<td>KOUNO, Ryou 16</td>
</tr>
<tr>
<td>KUBOTA, Yasuhiro 22</td>
</tr>
<tr>
<td>KUBOTA, Yuzuru 48</td>
</tr>
<tr>
<td>KUMA, Keichi 66</td>
</tr>
<tr>
<td>KUNICHIOKA, Sango 83</td>
</tr>
<tr>
<td>KUNIYOSHI, Minoru 16</td>
</tr>
<tr>
<td>KURAHASHI, Kensei 30</td>
</tr>
<tr>
<td>KURATA, Atsushi 34</td>
</tr>
<tr>
<td>KURATA, Hiroki 48</td>
</tr>
<tr>
<td>KURATA, Michio 84</td>
</tr>
<tr>
<td>KURIHARA, Tatsuo 34,79</td>
</tr>
<tr>
<td>KUROKAWA, Suguru 34</td>
</tr>
<tr>
<td>KUSAKA, Yasuhiro 28</td>
</tr>
<tr>
<td>KUSUDA, Toshie 18,78</td>
</tr>
<tr>
<td>KUSUMOTO, Tomoo 8</td>
</tr>
<tr>
<td>KUWAMOTO, Kiyoshi 48</td>
</tr>
<tr>
<td>Name</td>
</tr>
<tr>
<td>-----------------------</td>
</tr>
<tr>
<td>TAKAGI, Jumpei</td>
</tr>
<tr>
<td>TAKAHARA, Keigo</td>
</tr>
<tr>
<td>TAKAHASHI, Hideaki</td>
</tr>
<tr>
<td>TAKAHASHI, Hideroh</td>
</tr>
<tr>
<td>TAKAHASHI, Masahide</td>
</tr>
<tr>
<td>TAKAHASHI, Nobuaki</td>
</tr>
<tr>
<td>TAKAIJO, Daishi</td>
</tr>
<tr>
<td>TAKANO, Mikio</td>
</tr>
<tr>
<td>TAKASHIMA, Ryota</td>
</tr>
<tr>
<td>TAKASHIMA, Yohie</td>
</tr>
<tr>
<td>TAKATA, Kazuhide</td>
</tr>
<tr>
<td>TAKAYAMA, Yoshiyuki</td>
</tr>
<tr>
<td>TAKEDA, Nobuhiro</td>
</tr>
<tr>
<td>TAKEDA, Taijiro</td>
</tr>
<tr>
<td>TAKEDA, Yukio</td>
</tr>
<tr>
<td>TAKEHASHI, Masanori</td>
</tr>
<tr>
<td>TAKENO, Satoashi</td>
</tr>
<tr>
<td>TAKEUCHI, Ken-ichi</td>
</tr>
<tr>
<td>TAKEUCHI, Takeshi</td>
</tr>
<tr>
<td>TAKEUCHI, Toshihide</td>
</tr>
<tr>
<td>TAMADA, Yoshinori</td>
</tr>
<tr>
<td>TAMAO, Kobei</td>
</tr>
<tr>
<td>TANABE, Mikio</td>
</tr>
<tr>
<td>TANABE, Toshio</td>
</tr>
<tr>
<td>TANAKA, Hiroyuki</td>
</tr>
<tr>
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**[W]**

<table>
<thead>
<tr>
<th>Name</th>
<th>Page</th>
</tr>
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<tbody>
<tr>
<td>WADA, Ijao</td>
<td>38</td>
</tr>
<tr>
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</table>

**[Y]**

<table>
<thead>
<tr>
<th>Name</th>
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<tbody>
<tr>
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<td>48</td>
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<td>YAMAZAKI, Daisuke</td>
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<tr>
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<td>YAN, Wei</td>
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<td>YANAI, Kentaro</td>
<td>30</td>
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<td>YANG, Hu</td>
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<td>YAO, Junji</td>
<td>16</td>
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<td>32</td>
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<tr>
<td>YASUWA, Go</td>
<td>22</td>
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<td>16</td>
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<td>50</td>
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<tr>
<td>YOSHIDA, Hiroyuki</td>
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<tr>
<td>YOSHIDA, Kaname</td>
<td>48</td>
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<td>YOSHIDA, Ken</td>
<td>32</td>
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<tr>
<td>YOSHIDA, Konichi</td>
<td>22</td>
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<tr>
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<td>YOSHIKAWA, Chiaki</td>
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<tr>
<td>YOSHIMURA, Ken-ichi</td>
<td>56</td>
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<td>14</td>
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</tbody>
</table>

**[Z]**

<table>
<thead>
<tr>
<th>Name</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZHANG, Jian</td>
<td>16</td>
</tr>
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<td>ZHANG, Wanjiao</td>
<td>34</td>
</tr>
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<td>ZHU, Shangfeng</td>
<td>64</td>
</tr>
<tr>
<td>ZUSHI, Hirokazu</td>
<td>12</td>
</tr>
</tbody>
</table>
KEYWORD INDEX

[A] Alzheimer’s Disease 26  
Apoptosis 26  
Artificial Multilayers 18  
1-Aryltriazene 52  
Asymmetric Synthesis 8  
Australian Sector of the Antarctic Ocean 30

[B] Bacterial Cellulose 28  
Beam Cooling 44  
Beam Temperature 44  
Behavior 42  
Bioactive Trace Metals 30  
Bioinformatics 60, 64  
Biological Membrane 40

[C] Cell Morphogenesis 42  
Chemical State in Materials 50  
Chemoinformatics 62, 64  
π-Conjugated Systems 6  
COP9 Signalosome 24  
Cross-Coupling 52  
Cryptochrome 66  
Cyclometalated Radical 6  
Cytochrome P450 22

[D] D,L-Oligomer 8  
D-Amino Acid 34  
Data Mining 64  
Development of New Typed Spectrometer 50  
Dielectric Spectroscopy 38  
Diffusion 32  
Dissolved and Acid Dissolvable Species 30  
DNA Binding 20  
Drug Transport 32  
Dynamic Chirality 8

[E] E3 Ubiquitin Ligase 24  
EELS 48  
Electric Birefringence 38  
Electric Conductivity 54  
Electron Crystallography 48  
Electron Microscopy 14  
Electronic Structure Calculation 10  
Energetic Ion Generations 46  
Enzyme 34  
Enzyme Mechanism 22  
Epitaxial Growth 48

[F] Femtosecond Laser Spectroscopy 58  
Fallerene (Open-Cage) 6  
Fallerenylium Cation 6  
Functional Transition Metal Oxides 10

Genome 60  
Glass Structure 16  
Glycoinformatics 60  
Glycosidase 22  
Graph Algorithms 62

[H] Heterotaxia 4  
High Pressure Synthesis 54  
High Resolution TEM 48  
Higher Order Structure 36  
Highly Organized Materials 28  
Homogeneous Catalyst 56  
Homology Modeling 66

[I] Inorganic/Organic Hybrid Polymer 12  
Intracellular Delivery 20  
Iron-sulfur Cluster 34  
Isotactic Polypropylene 36

[K] KEGG 60  
Kernel Methods 62  
Kinetic Stabilization 4  
Kinetics 12

[L] Lipid Membrane 32  
Lipid Metabolism 42  
Living Radical Polymerization 12  
Low-coordinated Species 4

[M] Machine Learning 64  
Magnetic Ferroelectrics 10  
Magnetic Materials 18  
Magnetism 54  
Mass Spectrometer 46  
Membrane Lipid 42  
Mesomorphic Phase 36  
Microemulsion 40  
Molecular Evolution 66  
Molecular Recognition 8  
Multiple Alignment 66

[N] Nano Molecular Hybrids 28  
Nano-fabrication 18  
Nanoparticle 54  
Nano-structure Formation 46  
Natural Rubber 14  
Near-field Scanning 58  
Optical Microscopy 58  
Neutron Spin-echo 36  
NMR 32  
Nucleophilic Catalysis 8

[O] Oligosilane and Polysilane 52  
Organic EL Materials 28  
Organic Optoelectronic Device 40  
Organic-Inorganic Hybrid Low-Melting Glass 16  
Organosilicon Chemistry 52

[P] Parkinson’s Disease 26  
Pathway Analysis 60  
Peptide Engineering 20  
Phenypropanoid 22  
Photocatalysis 16  
Photoemission Spectroscopy 40  
Photomorphogenesis 24  
Photophysical Properties 52  
Photorefractive 16  
Phylogenetic Tree 66  
Poly(ADP-ribose)ylation 26  
Polymer Brush 12  
Polymer Gels 14, 36  
Polymer Solidolyte 14  
Precise Structure Analysis 10  
Protein Degradation 24  
Proteome 64  
Psychrophilic Bacterium 34

[R] Reaction Mechanism 56  
Rheology 38  
Rheo-Optics 38

[S] Scale-free Networks 62  
Scanning Probe Microscope 48  
Seawater 30  
Selenium 34  
Semiconductor Nanoparticles 58  
Septin 26  
Signal Transduction 24  
Silylum Ion 6  
Small Ring System 4  
Solenoid 44  
Sol-Gel Melting 16  
Solid-State NMR 28  
Spintronics 18  
Steric Protection 4  
Structural Biology 50  
Structural Comparison 50  
Sula Sea 30  
Super-strong Permanent Magnet 44  
Surface Grazing 12  
Systems Biology 62

[T] Thermoregulation 42  
Thin Layer Fabrication 54  
Toroid 44  
Transition Metal Clusters 56  
Transition Metal Complex 56  
Transition Metal Oxides 54
Transition
  Metal-Catalyzed Polymerization  36
  Transition-state Analog Inhibitors  22
  Transparent Electrode  40

  [U]
  Ultra-intense Laser  46
  Ultra-short Laser  46

  [W]
  Water-Gas-Shift Reaction  32

  [X]
  X-ray Diffraction  14
  X-ray Structural Analysis  50

  [Z]
  Zinc Finger Protein  20