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ICR ANNUAL REPORT 2004



Institute for Chemical Research Kyoto University

Volume 11

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

Unlais Tabaud

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, biogeochemistry in the hydrosphere, and biotechnology with useful enzymes and microorganisms.

Environment

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.

Functional Materials

International Research Center for Elements Science

Proposal of a guideline for creation of novel elementary materials through the uncovering of role of key elements which determine the functions of materials.

Elementary Materials

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 am ong chemistry, physics and biology. In cooperation with other divisions and centers in our institute, we will develop exploratory basic researches for founding advanced materials science.

Unification

Division of Biochemistry

Biology meets Chemistry; elucidating the mechanisms behind intra/inter-cellular recognition, stimuli response, and biomolecular synthesis in living matters for pioneering novel materials.

Bioscience

Bioinformatics Center

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

Genome

Division of Materials Chemistry

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

Nanomaterials

Advanced Research Center for Beam Science

Development of new capabilities with combination of various beams, Development of new method for space-time analysis with extreme resolution, Multidimensional analysis of functional chemical materials oriented for application, and Preparation for collaborative research scheme.

Extreme Conditions

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"



Director of ARBS: Prof NODA, Akira

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 Sasao, 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.scl.kyoto-u.ac.jp/~sakabe/ARBS-Home.html

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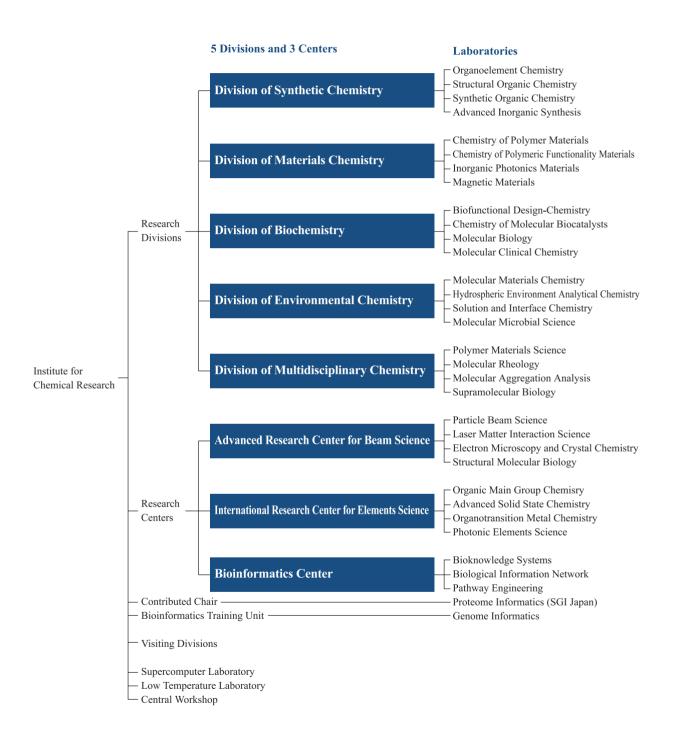
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– **A**bbreviations used in the columns

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

ORGANIZATION



(Reorganized on April 2004)

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry - Organoelement Chemistry -

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



Prof (D Sc)



Assoc Prof TOKITOH, Norihiro NAKAMURA, Kaoru (D Sc)



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Assist Prof TAKEDA, Nobuhiro (D Sc)



Assist Prof SASAMORI, Takahiro (D Sc)



Techn



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HAMAKI, Hirofumi (D1) HOSHINO, Wataru (M2) MIEDA, Eiko (M2) OZAKI, Shuhei (M1) KAWAI, Masahiro (M1) TANABE, Taro (M1)

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

Synthesis, Structures and Reactivities of Kinetically Stabilized Germaaromatic Compounds, Tokitoh N, Nakata N, Takeda N, The 11th International Conference On the Coordination and Organometallic Chemistry of Germanium, Tin and Lead, 27 June - 2 July 2004, Santa Fe, New Mexico, U.S.A.

Synthesis of Polythioethers Tethered with Bulky Aryl Groups and Their Complexation with Late-transition Metals, Tokitoh N, Shimizu D, Takeda N, Sasamori T, The 21st International Symposium on the Organic Chemistry of Sulfur, 4 - 9 July 2004, Madrid, Spain.

Synthesis of Silylboranes by the Reactions of a Bulky Silylene with Boron Compounds and Their Application to the Synthesis of a Borylsilyl Anion, Takeda N, Kajiwara T, Sasamori T, Tokitoh N, Heron Island Conference on Reactive Intermediates & Unusual Molecules, 17 - 23 July 2004, Queensland, Australia.

Syntheses and Properties of Transition Metal Complexes of Kinetically Stabilized Metallaaromatic Species of Heavier Group 14 Elements, Tokitoh N, The 36th International Conference on Coordination Chemistry, 18 - 23 July 2004, Merida, Mexico.

Generation and Reactions of Overcrowded Dimetallastannane Derivatives, Tajima T, Takeda N, Sasamori T, Tokitoh N, The 7th International Conference on Heteroatom Chemistry, 20 -25 August 2004, Shanghai, P. R. China.

Grants

Tokitoh 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.

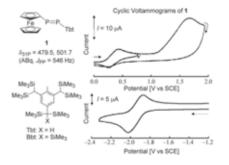
Tokitoh N, Synthesis of dynamic complexes containing heteroatoms by taking advantage of kinetic stabilization, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2002 - 31 March 2006.

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

Synthesis of the First Stable Ferrocenyldiphosphene and Elucidation of its Redox Behavior

A number of examples of kinetically stabilized diphosphenes (RP=PR), and diarsenes (RAs=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., distibene (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-tbutylphenyl), 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 TbtP=PFc and revealed its unique multi-switchable electrochemical prop-

Diphosphene 1 was synthesized by the dehydrochlorination reaction of Tbt-P(H)-P(Cl)-Fc with DBU. In sharp contrast to Mes*P=PFc, 1 is very stable in the solid state and even in solution. The molecular structure of 1 was confirmed by NMR spectra and X-ray crystallographic analysis, which evidenced the P=P double-bond character



of 1. The cyclic voltammograms of 1 showed the reversible reduction and oxidation couples at -1.91 and +0.34 V vs. SCE, respectively. The electrochemical results for 1 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)]₂ [3, pin = pinacolato] was achieved via the insertion reaction of 2 with bis(pinacolato)diboron. These reactions are quite important from the standpoints of development on a new synthetic method for borylsilanes and elucidation of reactivities of silvlenes. 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.

$$\begin{array}{c} \text{Tbt} \quad \text{Si:} \quad \begin{array}{c} \text{X-BR}_2 \\ \text{Mes} \\ \text{X} \\ \text{Si:} \\ \text{Mes} \\ \text{X} \\ \text{Si:} \\ \text{Mes} \\ \text{X} \\ \text{Mes} \\ \text{X} \\ \text{B(pin)} = -B \\ \text{B(pin)} \\ \text{B(pin)} \\ \text{B(pin)} \\ \text{B(pin)} \\ \text{B(pin)} \\ \text{Mes} \\ \text{B(pin)} \\ \text{Mes} \\ \text{Si} \\ \text{Mes} \\ \text{Mes} \\ \text{Si} \\ \text{Mes} \\ \text{Mes} \\ \text{Si} \\ \text{Mes} \\ \text$$

April 2003 - 31 March 2004.

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

Takeda N, Synthesis of double bond species between group 10 metals and chalcogens and the elucidation of their properties, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.

Sasamori T, Synthesis of novel π electron conjugated systems containing heavier group 14 and 15 elements and the elucidation of their properties, Grant-in-Aid for Young

Scientists (B), 1 April 2004 - 31 March 2006.

Nagahora N, Syntheses, structure, and properties of novel low-coordinated species of heavier main group elements, Grant-in-Aid for JSPS Fellows, 1 April 2003 - 31 March 2005.

Awards

Kajiwara T, Shinohara A, The Best Oral Presentation Award, The 84th Annual Meeting of the Chemical Society Japan, 27 April 2004.

Sugiyama Y, The Best Poster Award, The 17th Symposium on Fundamental Organic Chemistry, 25 September 2004.

Division of Synthetic Chemistry - Structural Organic Chemistry -

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



(D Eng)



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Assist Prof (D Eng)



Assist Prof MURATA, Yasujiro (D Eng)



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PD NOGITA, Rika (D Sc)



PD GAO, Yunyan (DSc)



PD MINEGISHI, Shynya (Ph D)

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MATSUBARA, Hiroaki (M1) TANINO, Nobuhide (UG) YOSHIDA, Ryohei (UG)

Scope of Research

Fundamental studies are being conducted for creation of new functional materials with novel structures and properties. The major subjects are: synthetic and structural studies on novel cyclic π-conjugated systems, particularly the positively charged species stabilized by σ - π interaction; synthesis of new redox-active and supramolecular π -systems; organochemical transformation of fullerenes C₆₀ and C₇₀, specifically the synthesis of open-cage fullerene derivatives and introduction and encapsulation of small molecules in the fullerene cage; generation of alkylated C₆₀ and C₇₀ cations and their application for the synthesis of functional materials.

Research Activities (Year 2004)

Presentations

Organic Functionalization of C₆₀ Toward Synthesis of Endohedral Fullerene, Komatsu K, Murata Y, Murata M, The 205th Meeting of The Electrochemical Society, 12 May, San Antonio, USA.

Alkylated Fullerenyl Cations: Their Generation, Isolation, and Stability, Kitagawa T, Lee Y, Masaoka N, Komatsu K, 17th IUPAC Conference on Physical Organic Chemistry, 18 August, Shanghai, P. R. China.

Sterically Segregated Cationic Oligothiophenes, Nishinaga T, Yamazaki D, Wakamiya A, Komatsu K, 6th International Symposium on Functional π -Electron Systems, 14 June, Ithaca, USA.

Synthesis and Properties of Open-Cage Fullerene C₇₀ Derivatives, Murata Y, Maeda S, Murata M, Komatsu K, The 205th Meeting of The Electrochemical Society, 12 May, San Antonio, USA.

Grants

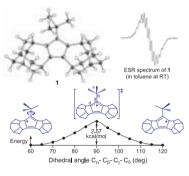
Komatsu K, Grant-in-Aid for Scientific Research (B), Development of Organic Synthetic Method for Endohedral Fullerenes, April 2004 - March 2006.

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

Spin-Localized Cyclopentadienyl Radical

A cyclopentadienyl radical 1, 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 anion 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-cyclopentadien-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

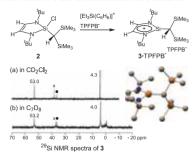
uniformly substituted cyclopentadienyl radicals, thus displaying the distinctive effect of annelation with rigid homoadamantene frameworks on the nature of cyclic π -conjugated systems.



A New π -Conjugated Silvlium Ion

Novel cationic silaaromatics, 2-silaimidazolium cation 3 was synthesized by chloride abstraction from the corresponding chlorosilane 2 with $[Et_3Si(benzene)]^+TPFPB^-$ (TPFPB- = tetrakis(pentafluorophenyl)borate) [2]. Cation 3 exists as a free silylium cation 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

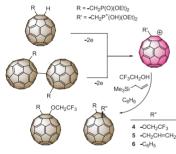
electronic effects of $6-\pi$ aromaticity and C–Si hyperconjugation are effective for stabilization of cation 3.



Generation of Fullerenyl Cation (EtO)₂P⁺(OH)CH₂-C₆₀⁺

Fullerenes are typically electronegative molecules, and only a few examples are known for their cations. Nevertheless, a novel fullerenyl cation, $(EtO)_2P^+(OH)CH_2-C_{60}^+$, was quantitatively generated by simply dissolving RC_{60} -H or RC_{60} - $C_{60}R$ ($R = CH_2P(O)(OEt)_2$) in H_2SO_4 . The cation was also generated in CD_2Cl_2 by the reaction of RC_{60} -H or RC_{60} - $C_{60}R$ with $(2,4-Br_2C_6H_3)_3N^{-+}SbF_6^-$. 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].



- [1] Kitagawa T, Ogawa K, Komatsu K, J. Am. Chem. Soc., 2004, 126, 9930.
- [2] Ishida S, Nishinaga T, West R, Komatsu K, Chem. Commun., 2005, 778.
- [3] Murata Y, Cheng F, Kitagawa T, Komatsu K, J. Am. Chem. Soc., 2004, 126, 8874.

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

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

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

Murata Y, Komatsu K, Academic-Industrial Cooperative Research Fund, April 2004 - March 2005.

Awards

Nishinaga T, Konica Minolta Technology Center Award

in Synthetic Organic Chemistry, Japan, Development of Molecular Wire Insulated by Rigid Carbon-Frameworks and Evaluation of Redox-Based Switching Properties, The Society of Synthetic Organic Chemistry, Japan, 18 February 2004.

Murata Y, The Chemical Society of Japan Award for Young Chemists, Novel Structural Transformation of Fullerene C₆₀, The Chemical Society of Japan, 27 March 2004.

Division of Synthetic Chemistry - Synthetic Organic Chemistry -

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Assist Prof TSUBAKI, Kazunori (D Pharm Sc)



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Visitors

Prof CLAYDEN, Jonathan Prof KAGAN, Henri Boris

Department of Chemistry, University of Manchester, England, 26 March, 2004 Institut de Chimie Molculaire 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 homooxacalixarene 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.

Preparation and Properties of C₂-Symmetric Chiral PPY Analogues, SCHEDEL H, KAWABATA T, 15th International Conference on Organic Synthesis (IUPAC ICOS-15), 5 August.

Asymmetric Synthesis of Nitrogen-Containing Heterocycles via Memory of Chirality, KAWABATAT, MAJUMDAR S, KAWAKAMI S, The 14th International Symposium on Fine Chemistry and Functional Polymer, 18 August.

Construction of Variable Temperature Visual Read Out

System for Sodium and Potassium Ions, TSUBAKI K, TANIMA D, KAWABATA T, International Conference on Supramolecular Science & Technology 2004, 9 September.

An Artificial Potassium Ionophore Based on D,L-Oligoester Architecture, KAWABATA T, OKAZAKI A, HIGASHINO I, 30th Symposium on Progress in Organic Reactions and Synthesis, Japan, 20 October.

Grants

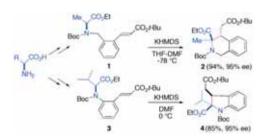
Kawabata T, Design of a New Generation of Nucleophilic Catalysts and Selective Reactions, Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2005.

Kawabata T, Development of C₂-Symmetric Chiral Nucleophilic Catalysts and Use in Asymmetric C-C Bond Formation, Grant-in-Aid for Scientific Research, 25 June 2004 - 24 June 2006.

Kawabata T, Asymmetric Cyclization based on the

A Novel Route to Highly Substituted Nitrogen Heterocycles from α -Amino Acids

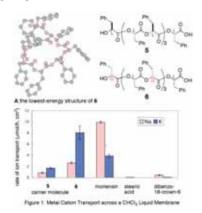
Nitrogen-containing heterocycles constitute important pharmacophore for drug discovery, useful building blocks for natural product syntheses, and the key structural subunits in asymmetric catalysis. We developed a novel route to highly substituted nitrogen heterocycles from readily available α -amino acids. Treatment of 1 with potassium hexamethyldisilazide (KHMDS) at -78°C gave tetrahydroisoquinoline 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.



An Artificial Potassium Ionophore Based on D,L-Oligoester Architecture

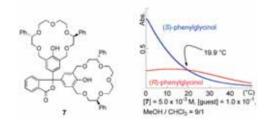
Homochiral oligoesters such as an oligolactate preferentially form a helical structure. On the other hand, D,L-oligolactate, consisting of alternating D- and L-lactic acid, favorably adopt a higher-ordered cyclic structure when lactic units are in the range of 6~8. Structural analysis indicated that the cyclic structure of these D,L-oligolactate is not the result from intramolecular hydrogen-bonding, but from their D,L-chirality. Ion-transport experiments were performed with octaesters 5 and 6 consisting of 2-hydroxy-3-phenylpropionic units. D,L-Octaester 6 showed the higher rate of ion transport both for Na⁺ and K⁺ than the corresponding homochiral octaester 5. Potassium ion was

selectively transported by **6** and the rate was much higher than that by dibenzo 18-crown-6 and comparable with that of sodium-ion transport by a well-known ionophore, monensin. These properties of **6** seem to originate from its cyclic preorganized structure **A**.



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 (AITs) 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.



Dynamic Chirality of Enolates, Grant-in-Aid for Scientific Research, 31 October 2002 - 30 October 2004.

Awards

TSUBAKI Kazunori, The Society of Synthetic Organic

Chemistry, Japan, Kansai Branch Award, 19 November 2004.

MONGUCHI Daiki, Best Poster Award, 21st Summer School of Synthetic Organic Chemistry, 14 July 2004.

Division of Synthetic Chemistry- Advanced Inorganic Synthesis -

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Prof SHIMAKAWA, Yuichi (D Sc)



Assoc Prof AZUMA, Masaki (D Sc)



Assist Prof IKEDA, Yasunori



PD (PRESTO)
BELIK, Alexei A.
(D Sc)

Students

KANDA, Hironori (D3) NAKAMURA, Motonori (RF)

Visitor

Dr SUBRAMANIAN, Mas 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

Structure and physical properties of Pb-3d transition metal perovskites, A. A. Belik, M. Azuma, and M. Takano, 2004 Spring JPS annual meeting, Fukuoka, Japan, 27 March 2004.

New perovskite-type oxides with possibly large ferroelectric polarizations, Y. Shimakawa, S. Niitaka, A. A. Belik, M. Azuma, and M. Takano, 2004 Autumn JSAP 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.

Noncentrosymmetric Bi, Pb-3d transition metal perovskites, M. Azuma, S. Niitaka, A.A. Belik, S. Ishiwata, K. Takata, H. Kanda, I. Yamada, Y. Shimakawa, and M. Takano, Fourth International Conference on Inorganic Materials, Antwerp, Belgium, 20 September 2004.

Diverse magnetic properties among low-dimensional

 $BaMP_2O_7$ (M = Co, Ni, and Cu) and $BaCuV_2O_7$, A.A. Belik, M. Azuma, and M. Takano, Fourth International Conference on Inorganic Materials, Antwerp, Belgium, 20 September 2004.

A Designed New Ferromagnetic Ferroelectric Bi₂NiMnO₆, M. Azuma, K. Takata, M. Hashisaka, T. Saito, T. Terashima, K. Mibu, Y. Shimakawa, and M. Takano, The 4th International Workshop on Novel Quantum Phenomena in Transition Metal Oxides, Sendai, Japan, 22 November 2004.

Grants

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

Azuma M, Exploration of Photo-Functions in Strongly Correlated Electron Systems of Transition Metal Oxides, PRESTO, 1 December 2001 - 31 March 2005.

High-Pressure Synthesis of PbVO₃ - A New Member of PbTiO₃ 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. PbTiO₃ is a well known ferroelectric with a large spontaneous polarization, P_s , of 81 μ C/cm² at room temperature. Existence of the $6s^2$ lone electron pair of Pb²⁺ ion and the orbital hybridization between the Pb 6s state and O 2p states in PbTiO₃ 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., BaTiO₃.

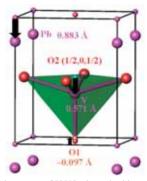


Figure 1. Crystal structure of PbVO₃ determined by means of synchrotron X-ray powder diffraction study. Heavy atomic displacements give rise to a large spontaneous polarization.

PbTiO₃ is the only simple perovskite oxide with the composition PbMO₃ (*M* is a transition metal) which can be prepared at ambient pressure. We found that a new perovskite-type oxide PbVO₃, isotypic with PbTiO₃, 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 PbVO₃ among the reported PbTiO₃-type materials that suggests a large polarization of PbVO₃.

A Designed New Ferromagnetic Ferroelectric Compound Bi₂NiMnO₆

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 $\mathrm{Bi^{3+}}$ or $\mathrm{Pb^{2+}}$ ions with magnetic transition metal ions in a perovksite structure so that the $6s^2$ lone pair of $\mathrm{Bi^{3+}}(\mathrm{Pb^{2+}})$ 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.

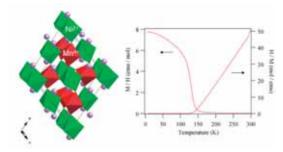


Figure 2. Crystal structure (left) and the magnetic susceptibility data (right) of Bi_2NiMnO_6 . NaCl type distribution of Ni^{2+} and Mn^{4+} ions is the origin of the ferromagnetism.

A designed ferromagnetic ferroelectric double provskite Bi₂NiMnO₆ was prepared by means of high-pressure synthesis. The noncentrosymmetric structure and the ordering of Ni²⁺ and Mn⁴⁺ 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 Bi₂*M*²⁺*M*³⁺*M*³⁺O₆ and Pb₂*M*³⁺*M*³⁺O₆ systems (*M*: magnetic transition metal) for further finding of new magnetic ferroelectric compounds.

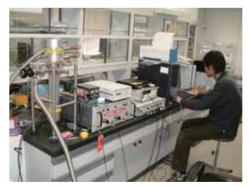


Figure 3. K. Takata working on the ferroelectric property measurement system.

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Visitors

Dr TONGE, Mathew Prof MIYATA, Seizo Prof WATANABE, Junji Mr LADMIRAL, Vincent R. Prof HAN, Yanchun Prof MÜLLER, Axel H. E.

Stellenbosh University, South Africa, 3 February 2004

President, Tokyo University of Agriculture and Engineering, 28 May 2004

Tokyo Institute of Technology, 28 May 2004

University of Warwick, UK, 6 July - 23 August 2004 Chinese Academy of Sciences, China, 17 November 2004 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 Property of HDPB (Invited Lecture), Tsujii Y, UK-JPN Polymer Workshop 2004, Kyoto, 1 - 2 April.

Precision Design and Application of Organic/Inorganic Hybrid Particles Coated with HDPB (Invited Lecture), Ohno K, and 7 other presentations, 53rd Spring Meeting, Soc. Polym. Sci., Jpn., Kobe, 28 - 30 May.

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.

Surface Modification by LRP (Invited Lecture), Fukuda T, 51st Summer College, Soc. Polym. Sci., Jpn., Oshima, 12 - 14 July.

4 presentations, 50th Polymer Symposium, Soc. Polym.

Sci., Jpn., Kobe, 15 July.

2 presentations, 2nd Trilateral Workshop on Organic Chemistry, Kyoto, 4 - 6 September.

4 presentations, 53rd Autumn Meeting, Soc. Polym. Sci., Jpn., Sapporo, 15 - 17 September.

Structural Studies of HDPB by Neutron Reflectometry (Invited Lecture), Tsujii Y, 4th Annual Meeting of Jpn. Soc. Neutron Sci., Sapporo, 16 - 17 December.

Grants

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

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

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 ($X = SbMe_2$) 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 $C_{\rm ex}$ significantly depended on polymers, increasing in the order of methyl methacry-

late < styrene < methyl acrylate. For the SBRP of styrene, DT was the only important activation mechanism. The $C_{\rm ex}$ was about twice as large as that for the TERP of styrene, explaining why the SBRP has a better polydispersity controllability than the TERP.

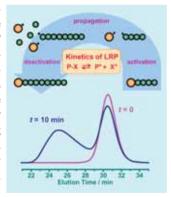


Figure 1. Schematic representation showing the activation, propagation, and deactivation processes in LRP (top) and the evolution of chain length and chain length distribution as followed by GPC (bottom). The activation rate constant was determined by following the decay of the dormant species concentration 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).

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

Incompletely condensed polyhedral oligomeric silsesquioxane with the highly reactive group of trisodium silanolate was used for the synthesis of two initiators for atom transfer radical polymerization, one with a 2-bromoisobutyl group (7Ph-T₈-BIE), and the other with a chlorosulfonyl group (7Ph-T₈-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.

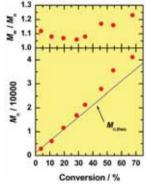


Figure 2. Evolution of number-average molecular weight (M_n) and polydispersity index (M_w/M_n) of POSS-PMMAs as a function of monomer conversion for the solution polymerization of MMA (50 wt %) in anisole at 70°C with 7Ph-T₈-CSPE. The full line in Figure 2 represents the theoretical prediction calculated as the molar ratio of polymerized monomer to the initiator.

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

Tanaka K, Construction of Nanoelectronic Devices,

CREST, Jpn. Sci. Tech. Corp., 1 November 2002 - 31 October 2007.

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

Ohno K, Magnetically Tunable Colloidal Crystal, ICR Collaboration, 2004.

Division of Materials Chemistry - Chemistry of Polymeric Functionality Materials -

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Visitors

Dr SCHAPER, Andreas Dr TRACZ, Adam

Philipps University in Marburg, Germany, 25 January - April 18 2004

Center of Molecular and Macromolecular Studies, Polish Academy of Sciences,

Poland, 12 March 2004

Mr WU, Ming-Chien Prof FAN, Zenglu

National Cheng Kung University, Taiwan, 5 July - 30 August 2004

Xi'an University of Engineering Science and Technology, P.R. China 5 August

2004 - 29 January 2005

Dr KRACOVSKY, Ivan Prof ISMAIL, Hanafi

Charles University, Czech Republic, 30 August 2004 - 30 June 2005

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 higherorder 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 crystallization of natural rubber, (2) Ionic conductivity of uniaxially stretched elastomer, (3) Direct observation of molecular chains in the epitaxially grown lamellar crystals of polymers, 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 presen-

"Keynote: Dynamical studies on strain-induced crystallization of natural rubber vulcanizates using a synchrotron X-ray source", Kohjiya S, 4th International Materials Technology Conference & Exhibition (IMTCE2004), Kuala Lumpur, Malaysia, 23-25 March and other 1 presentation.

"3-D TEM and AFM observations of silica generated in situ in natural rubber", Kohjiya S, Katoh A, Shimanuki J, Hasegawa T, Ikeda Y, The 165th Spring Technical Meeting of Rubber Division, ACS, Grand Rapids, Mishigan, USA, 17-19 May.

"Preparation of nanocomposites composed of highly crystalline cellulose microfibrils and imogolite", Ikuno M, Hirai A, Horii F, Donkai N, Tsuji M, 53rd Spring Meeting, The Society of Polymer Science, Japan, Kobe, 25-27 May and other 6 presentations.

"Electron crystallography on beam sensitive materials - Part 1 and 2", Tsuji M, Invited lecture, International

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.

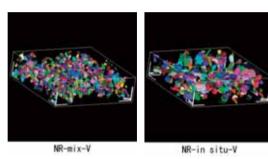


Figure 1. Colored volume rendered 3D views of the reconstructed mass density distribution of the silica inclusions for NR-mix-V and NR-in situ-V after removal of zinc compounds. The individual silica particles and aggregates were isolated from the neighbors by coloring. The frame is shown in reconstructed perspective geometry (length and width: 630 nm, thickness: 181 nm). The bar for each direction shows the distance of 100 nm.

Ionic Conductivity of Uniaxially Stretched Poly(oxyethylene)s

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)s (PEO) on ionic conductivity. From the relationship between the lithiumion 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 continually with an increase of the stretching ratio.

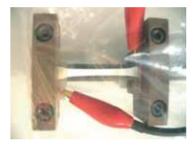


Figure 2. Ionic conductivity measurements with uniaxially stretched PEO.

School of Crystallography, 36th Course, "Electron Crystallography: Novel approaches for structure determination of nanosized materials", Erice-Sicily, Italy, 9-20 June.

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

"3D-TEM observation of in situ silica in natural rubber matrix", Kohjiya S, Ikeda Y, Katoh A, Shimanuki J, Sawabe H, Gonda M, Suda T, Kojima N, Nishioka M, Hasegawa T, 53rd Autumn Meeting, The Society of Polymer Science, Japan, Hokkaido, 15-17 September and other 4 presentations.

"Crystalline morphologies of unoriented and uniaxially oriented thin films of poly(butylene terephthalate) (PBT)", Yoshioka T, Tsuji M, Fujimura T, and Kohjiya S, 14th Symposium on Polymeric Materials, Kyoto, 1 December and other 1 presentation.

"Strain-induced crystallization in filled natural rubber vulcanizates", M, Poompradub S, Tosaka M, Murakami S, Kohjiya S, Ikeda Y, Toki, S, Sics I, Hsiao, B S, 17th Meeting on Elastomer (The Society of Rubber Industry, Japan), Kobe, 2-3 December and other 3 presentations.

Grants

Kohjiya S, Stress-induced crystallization behavior of natural rubber, Grant-in-Aid for Scientific Research, (B) (2), 1 April 2003 - 31 March 2005.

Tsuji M, High-resolution TEM of the shish-kebab structure in uniaxially oriented polyesters, Grant-in-Aid for Scientific Research, (C) (2), 1 April 2004 - 31 March 2007.

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 -

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Prof (D Eng)



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Assist Prof (D Eng)



MENAA, Bouzid (PhD)



PD YAO, Jianxi (Ph D)



KAKIUCHIDA, Hiroshi (D Eng)



PD KANG, Eun-Seok (PhD)



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KOUNO, Ryou (UG) SUZUKI, Masaru (UG) FUJII, Masao (UG) FUKUDA, Masahiro (RF) FUKUDA, Masaaki (RF) KUNIYOSHI, Minoru (RF) 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-resoluction NMR, thermal analysis, various laser spectroscopies and ab initio molecular orbital calculations.

Research Activities (Year 2004)

Presentations

Na environment in sodium silicate glasses by ²³Na 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 hybrid low-melting glasses for photonics 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_{4-m}SiO_{m/2} units, Kakiuchida H, Takahashi M, Masai H, Tokuda Y, and Yoko T, ibid.

Preparation and properties of organic-inorganic hybrid low-melting glass films, Bouzid M, 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 ionic heater, Takahashi M, Saito 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 lowmelting glass of SnO-Me₂SiO_{2/2}-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 H₃PO₄, or H₃PO₃ as Lewis acid and Si(CH₃)₂Cl₂, 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 nonirradiated part. The photoinduced refractive index change was estimated to be of the order of $\Delta n = -2 \times 10^{-3}$ with a

MZ interferometer. Moreover, we have succeeded in fabricating waveguide or phase grating structures inside the hybrid lowmelting glass as shown in Fig.1.

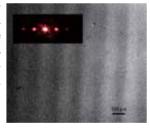


Figure 1. Phase grating structure written inside the low-melting glasses by laser heating through nonradiative phonon emission of an excited rare earth ion. Inset shows the diffraction of He-Ne laser light by the phase grating. (The higher order diffractions are also clearly observed)

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.

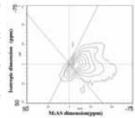


Figure 2. ²³Na MQMAS spectrum of Na₂O-2SiO₂ glass. MAS dimension and isotropic dimension are presented in ppm relative to an external reference of 1 mol/L NaCl solution. Inset two lines represent chemical shift (QS) and quadrupolar interaction shift (QIS).

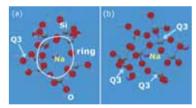


Figure 3. Optimized clusters modeling (a) isolated Na ion and (b) crowded one. The calculated chemical shifts of model (a) and (b) are 566.2 and 566.6 ppm, respectively. The quadrupolar shifts are calculated as 0.5 and 3.2 ppm for model (a) and (b), respectively. All these calculations were performed at the HF/6-31G* level.

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, Grantin-Aid for Scientific Research (A) (2), 1 April 2001 - 31 March 2005.

Yoko T, Preparation of organic-inorgaic hybrid low-melting glasses through asid-base reaction, Asahi Glass Foundation, 1 April 2004 - 31 March 2005.

Yoko T, Optical measurement of glass transition temperatures, New Glass Forum, 1 April 2002 - 31 March 2004.

Takahashi M, Development of photorefractive low-

melting glasses, Grant-in-Aid for Scientific Research (B) (2), 1 April 2001 - 31 March 2005.

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

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

Takahashi M, Murata Scientific Foundation, 1 July 2004 - 31 June 2005.

Yao J, Preparation of porous TiO₂ electrodes by photo-induced phase separation technique, Grant-in-Aid for Scientific Research for JSPS Researcher, 1 April 2004-31 March 2005.

Division of Materials Chemistry- Magnetic Materials -

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



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Visitors

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

May 2004

Prof HAESENDONCK,C. Laboratoratory 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/Nanotechnology, 3 - 5 March 2004, Sendai, Japan.

Dynamics of a magnetic domain wall in magnetic wires, Ono T, International Conference on Nanospintronics Design and Realization, 24 - 28 May 2004, Kyoto, Japan.

Spin-dependent transport in ferromagnet/superconductor/ferromagnet double tunnel junctions, Miura K, Ono T, Nasu S, International Conference on Nanospintronics Design and Realization, 24 - 28 May 2004, Kyoto, Japan.

Dynamics of a magnetic domain wall in submicron magnetic wires with asymmetric notches, Himeno A, Okuno T, Ono T, International Conference on Nanospintronics Design and Realization, 24 - 28 May 2004, Kyoto, 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 Ni₈₁Fe₁₉/Al/ Ni₈₁Fe₁₉ double tunnel junctions, Miura K, Ono T, Nasu S, 5th International Symposium on Metallic Multilayers, 7 - 11 June 2004,

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 Seminor, 2 - 4 September 2004, Kobe Institute, Kobe, Japan.

Direct observation of current-driven domain wall motion in magnetic nano-wires, Ono T, International Workshop on Materials Science and Nano-Engineering, 11 - 14 December 2004, Osaka, 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 6.7×10^{11} A/m² and 0.5 µs, 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 pulsedcurrent.

Yamaguchi A., Ono T., et al., Phys. Rev. Lett., 92 (2004) 077205.

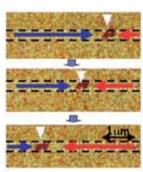


Figure 1. Real-space observation of the current-driven domain wall motion by a magnetic force microscopy.

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 Ni₈₁Fe₁₉/Al/ Ni₈₁Fe₁₉ 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 Al/Al₂O₃/ Ni₈₁Fe₁₉ tunnel junctions at the overlap of the Al wire and the Ni₈₁Fe₁₉ wires. A current *I* enters from the left Ni₈₁Fe₁₉ electrode and is extracted at the left end of the Al wire. Spin polarized electrons injected from Ni₈₁Fe₁₉ into Al create nonequilibrium spin accumulation in Al. This spin accumulation is detected as voltage V measured between the right Ni₈₁Fe₁₉ 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 Ni₈₁Fe₁₉ 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 Ni₈₁Fe₁₉ electrodes changes from parallel to anti-parallel, indicating the exis-

tence of the difference in electrochemical potentials between the spin-up and spin-down electrons injected from Ni₈₁Fe₁₉ into the Al wire.

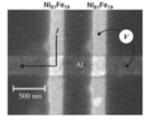


Figure 2. SEM image of the spin injection and detection device, with the geometry of the non-local measurement.

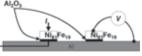
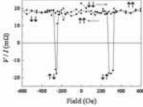


Figure 3. Spin-signal $\emph{V/I}$ for $Ni_{81}Fe_{19}/Al/Ni_{81}Fe_{19}$ as a function of magnetic field at 10 K.



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.

Ono T, Invention of anomalous quantum materials, Grant-in-Aid for Scientific Research in Priority Areas, 1 April 2004 - 31 March 2010.

Award

Yamaguchi A, Tanigawa H, Ono T, Nasu S, Miyake K, Mibu K, Shinjo T, MSJ Distinguished Paper Award, Current-driven domain wall motion due to the spin-transfer effect, Magnetics Society of Japan, 22 September 2004.

Division of Biochemistry - Biofunctional Design-Chemistry -

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Visitors

Prof VIVES, Eric Dr MIHALA, Nikolett University of Montpellier II, France, 16 February 2004

Research Group for Peptide Chemistry, Hungarian Academy of Sciences, Hungary, 27

July - 31 August 2004

Prof DIBO, Gabor Prof HUDECZ, Ferenc Institute of Chemistry, Eotvos L. University, Hungary, 22 October 2004

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 Seminor of Risbon University, Risbon, Prortogal, 15 March.

Structure and Function of Zinc Finger Proteins, Sugiura Y, 124th Annual Meeting of Pharmaceutical Sciences of Japan, Osaka, 29 March.

Delivery of macromolecules into cells using non-viral vectors, Arginine-rich peptides: aspects of membrane translocation, Futaki S, Molecular design in 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.

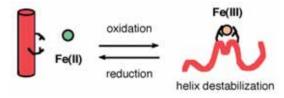
Grants

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 i and i+2 positions in a 17-redsidue 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 leucinezipper 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 peptidebased 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 C₂H₂-type zinc finger has a tandemly-repeated structure, which consists of independent modules with the consensus sequence, ((Tyr, Phe)-X-Cys-X₂,4-Cys-X₃-Phe-X₅-

Leu-X₂-His-X₃₋₅-His-X₂₋₆). Each domain forms a compact bba structure held together tetrahedrally by coordination of a zinc ion with two invariant cysteines and histidines. Typical C₂H₂-type zinc fingers recognize the three-basepair 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 C₂H₂-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 GLItype 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.

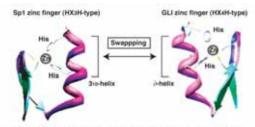


Figure 1: Swapping of histidine spacings between Sp1 and GLI zinc fingers.

multi-zinc finger protein, Sp1ZF15, Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 march 2006.

Futaki S, Functional design of cell-targeting peptides,

PRESTO program, Japan Science and Technology Agency, 1 November 2002 - 31 October 2005.

Division of Biochemistry - Chemistry of Molecular Biocatalysts -

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



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Visitors

Prof WAN, Xiao-chun, Prof XIA, Tao, Assoc Prof LI, Shangqing, Dr ZHANG, Zhengzhu 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 aglycons. 2) Molecular basis of the floral aroma formation in oolong tea. 3) Design and synthesis of transition-state analogue and mechanism-based inhibitors of γ-glutamyltranspeptidase. 4) Design and synthesis of novel inhibitors of glycosidases and their application as affinity chromatography and biological probes to understand the physiological roles of glycosidases. 5) Directed evolutional 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.

β-Glycosidase inhibitors: physicochemical properties of β-glycosylamidines and their mechanism of inhibition, Kato M, Hiratake J, Sakata K, 2004 Annual Meeting of Kansai Branch of Jpn. Soc. Biosci. Biotech., and Agrochem., Nagahama (Shiga), 3 October.

Design and synthesis of inhibitors of IAA-amino acid conjugate hydrolases, Kubota Y, Hiratake J, Mizutani M, Sakata K, 2004 Annual Meeting of Kansai Branch of Jpn. Soc. Biosci. Biotech., and Agrochem., Nagahama (Shiga), 3 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 (18O2). The sweet potato discs treated with chitosan (1 mg/ml) as an inducer were exposed to the artificial air consisted of N2, 18O2 and CO2 for 24 hr, and the accumulated umbeliferone was analyzed by ESI-LC/MS². 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/z107, 119, 135 on the MS² spectrum after N₂ 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 $^{18}\text{O}_2$, intensities of the ions m/z 165 and 167 were 80% and 74% weaker than those of the discs treated with ¹⁸O₂, respectively. The control discs incubated in H₂¹⁸O similarly gave weaker intensities of these ions, indicating ¹⁸O in the ions m/z 165 and 167 is not from H₂O. These data indicate that ¹⁸O₂ 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 O₂ (Figure 1).

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

Grants

Sakata K, (B) (2), 1 April 2004 - 31 March 2007.

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

Sakata K, Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2005.

Hiratake J, Grant-in-Aid for Scientific Research (B) (2),

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 activesite 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 oleoyl 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.

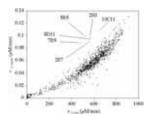


Figure 2. Amide- and ester-hydrolyzing activities (v_0 , amide and $v_{0, \text{ ester}}$) of mutant linases

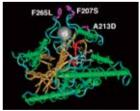


Figure 3. Structural model of lipase

1 April 2004 - 31 March 2007.

Mizutani M, Grant-in-Aid for Young Scientist B, 1 April 2003 - 31 March 2005.

Award

Saito S, The ICR Award for Young Scientist, ICR, 3 December 2003.

Division of Biochemistry - Molecular Biology -

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Res Associate OHASHI, Yohei (D Sc)



Techn YASUDA, Keiko



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Technician (pt) NAKAGAWA, Shuko

Visitors

Prof BANKAITIS, V.A. Prof OU, L.-J.

University of North Carolina, Chapel Hill, USA, 26 April 2004 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 AtPLD\(\mathcal{L}\)2 gene in Arabidopsis thaliana, Yamamoto Y, Ohashi Y, Oka A, Aoyama T, 2004 Ann Meeting of Jpn Soc Plant Physiol, 27 - 29 March (Hachioji).

Phospholipase D controlling plant cell morphogenesis, Aoyama T, 2004 Spring Symposium of Mol Biol Soc Jpn, 19 - 20 May (Nara).

Targets of ARR1, Aoyama T, International Workshop on Cytokinin Metabolisms, Signaling and Function, 10 July (Berlin, Germany).

Interaction between CSN1 (COP9 Signalosome subunit 1) and components of transcription/RNA processing complexes SAP130, DdX15/hPrp43/mDEAH9, and CFIm68, 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 (Suita).

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).

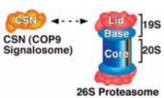
Hunting target genes of Arabidopsis transcription factors, Aoyama T, Workshop at University of Rome La Sapienza, 18 October (Rome, Italy).

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/fus* mutants possessing light grown seedling phenotype in the dark. The ten responsible *COP/DET/FUS* 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 evolutional relationship (left figure).

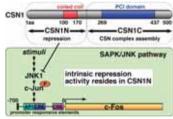
Individual subunits of the CSN has been linked to various signal pathways leading to gene expression regulation and cell cycle control.



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 Rub1 or animal NEDD8) and the Cullin subunit of the E3 ligase [1]. This

regulation through protein degradation eventually modulates the signal transduction pathways involved in cell cycle, morphogenesis, and stress response [2]. Further dissection revealed that the C-terminal half of CSN1 subunit, encompassing the PCI domain, is responsible for interaction with CSN2, CSN3, and CSN4 subunits and therefore required as a scaffold for CSN assembly as a complex. The N-terminal portion of CSN1 (CSN1N), on the other hand, possessed an intrinsic function of repression on gene expression. We found that CSN1N represses the SAPK/JNK (c-Jun N-terminal kinase) signaling pathway by suppressing the activated signal of the proto-oncogene c-Fos through its responsive elements on the promoter [3].

We further found that CSN1N potently reduces the accumulation of JNK1 protein in the cells leading to the suppression of c-Jun phosphorylation (right figure). However, this regulation of repression was independent from the known protein-degradation mediated regulation, as shown by several lines of circumstantial evidence. In belief that this regulation was caused through protein-protein interaction, we set out to identify interacting proteins that directly bind to CSN1N. We have isolated and identified a novel spectrum of interacting proteins (NBPs) supporting the above idea. To understand the biological roles of NBPs in the regulation of signal transduction on morphogenesis, we have constructed a series of knockout plants defective in each of the NBP gene, taking advantage of the various resources available in Arabidopsis. Detailed biochemical analyses on the CSN-NBP interactions in combination with in planta research will reveal the novel mechanism of CSN on signal transduction.



1. Science 292, 1382-5 (2001). 2. Curr Biol 12, 667-72 (2002). 3. J Mol Biol 305, 1-9 (2001).

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

regulatory system of phosphorelay 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 phosphorelay 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.

Division of Biochemistry - Molecular Clinical Chemistry -

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







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Students

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Scope of Research

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

Attenuation of Mitochondrial Impairment by Poly(ADP-ribose) Polymerase-1 siRNA in Experimental Models of Cerebral Ischemia and Reperfusion, Tanaka S, Takehashi M, and Ueda K, The 53rd Fujihara International Seminar, Tomakomai, 26 - 29 July.

Suppression of Oxidative Cell Death by Poly(ADP-ribose) Synthetase Inhibitors, Ueda K, Tanaka S, Takehashi M, Banasik M, and Stedeford T, The 53rd Fujihara International Seminar, Tomakomai, 26 - 29 July.

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.

Attenuation of Mitochondrial Injury by Poly(ADPribose) Synthetase siRNA in Experimental Model of Cerebral Ischemia, Tanaka S, Takehashi M, and Ueda K, Joint Meeting of the 27th Annual Meeting of the Japan Neuroscience Society and the 47th Annual Meeting of the Japanese Society for Neurochemistry, Osaka, 21 - 23 September.

Expression, Distribution, and Complex-Formation of Septin 3 Isoforms in Human Brain, Takehashi M, Tanaka S, Tsukagoshi-Nagai H, Kinoshita N, Kawamata T, Ueda K, 77th Annual Meeting of Japanese Biochemical Society, Yokohama, 13 - 16 October.

Poly(ADP-ribose) Polymerase-1 Activation and Mitochondrial Injury Determine the Pattern of Cell Death, Apoptosis or Necrosis, Tanaka S, Takehashi M, and Ueda K, 77th Annual Meeting of Japanese Biochemical Society, Yokohama, 13 - 16 October.

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 oxygenglucose 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-Reoxinduced 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, 1,5dihydroxyisoquinoline and benzamide. 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.

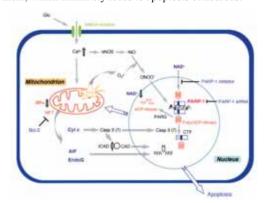


Figure 1. Molecular mechanism of neuronal apoptosis after cerebral ischemia.

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 tetra-

chloride (CCl₄). Male ICR mice treated via the intraperitoneal route with CCl₄ exhibited severe necrotic centrilobular lesions and significantly elevated serum transaminases. In contrast, the histopathology and serum biochemistry of animals treated concomitantly with CCl₄ and 6(5*H*)-phenanthridinone were not significantly different versus controls. In conclusion, the results of this study demonstrate that the hepatotoxicity of CCl₄ can be blocked independently of its metabolism and suggest the predominant role of PARP-1 overactivation in chemical-induced toxicity.

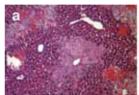




Figure 2. H-E stained liver sections from male ICR mice (200x). (a) CCl₄: severe necrosis in centrilobular regions with loss of hepatocyte morphology and prominent red cell extravasations into the necrotic areas. (b) CCl₄ + 6(5H)-phenanthridinone: normal hepatocyte morphology and liver architecture.

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.

Division of Environmental Chemistry - Molecular Materials Chemistry -

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



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Dr AMORNSAKCHAI, Taweechai Mr CHAIYUT, Nattawut

Donghua University, China, 1 - 11 July 2004, 18 - 26 October, 2004

Mahidol University, Thailand, 9 - 22 October 2004 Mahidol University, Thailand, 1 April - 31 August 2004

Scope of Research

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

Research Activities (Year 2004)

Presentations

Super-High Field Solid-State NMR for Structural Analyses of Advanced Materials, Horii F, 35th Solid-State NMR for Materials Meeting, 11 May (Invited).

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).

Preparation of Nanocomposites Composed of Highly Crystalline Cellulose Microfibrils and Imogolite, Ikuno M, Hirai A, Horii F, Donkai N, Tsuji M, 53rd Annual Meeting, Soc. Polym. Sci., Jpn., 25 May.

Dynamics of Hole-Transport Material in Organic EL Device, - Analysis of Dynamics by Two-Dimensional Solid-State ¹³C and ²H NMR Spectroscopy -, Tsukamoto N, Kaji H, Horii F, 53rd Annual Meeting, Soc. Polym. Sci., Jpn., 25 May.

Structure and Structural Change of Sub-elementary Fibrils of Bacterial Cellulose in an Initial Period of Organization, Suzuki F, Tsujitani K, Hirai A, Horii F, 53rd Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 16 September.

Cationic States of a Hole Transport Material in Organic EL Devices, -Analysis by Solid-State ¹⁵N, ¹³C NMR and Quantum Chemical Calculation-, Yamada T, Kaji H, Tsukamoto N, Kusaka Y, Horii F, 53rd Symposium on Macromolecules, Soc. Polym. Sci., Jpn., 15 September.

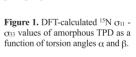
Grants

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

A Combined Experimental and Theoretical Study of the Conformation of TPD Using Solid-State ¹⁵N NMR and DFT Calculations

The conformation of N, N'-diphenyl-N, N'-di(mtolyl)benzidine (TPD) (Figure 1), which is widely used as a hole-transport material in organic electroluminescent (OEL) devices, has been studied by solid-state ¹⁵N 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 ¹⁵N NMR chemical shift anisotropy (CSA) spans, $\sigma_{11} - \sigma_{33}$, of amorphous TPD plotted as a function of the torsion angles, α and β . The CSA spans significantly vary depending on the conformation and can be used for the determination of torsion angles. The experimental CSA span of ¹⁵N-labeled amorphous TPD was 15 ppm. This corresponds to the narrowest CSA span among the DFT-calculated values in Figure. 1. The DFToptimized structure with torsion angles α of 40-41° and β 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.



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

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

Kaji H, Higher Order Structures and Optical Properties of Light-Emitting Polymeric Materials, PRESTO, Japan [1] H. Kaji, T. Yamada, N. Tsukamoto, F. Horii, Chem. Phys. Lett., 401, 246-253 (2005).

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.

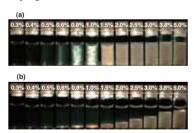


Figure 2. Phase behavior of microfibrils/imogolite nanotubes (1/1) dispersed in the aqueous solution of acetic acid as a function of the total concentration. (a) Immediately after preparation. (b) After 2 months. The turbid phase is the liquid crystalline phase. The concentration of the A point is 0.4%.

Science and Technology Agency, 1 November 2002 - 31 October 2005.

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

Division of Environmental Chemistry

- Hydrospheric Environment Analytical Chemistry -

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Visitor

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

Scope of Research

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

Research Activities (Year 2004)

Presentations

Dynamics of bioactive trace metals during the Subarctic Pacific Iron Experiment for Ecosystem Dynamics Study (SEEDS2001), Sohrin Y, Kinugasa M, Okamura K, Takeda S, Nishioka J, Tsuda A, Ocean Research Conference, 19 February 2004.

Development of analysis for suspended particulate metals in seawater and behavior of these elements in Subarctic Pacific Iron Experiment for Ecosystem Dynamics Study (SEEDS2001), Nakatsuka S, Kinugasa M, Sohrin Y, The 65th conference on the Japan Society for Analytical Chemistry, 15 May 2004.

Solvent extraction of divalent metal ions with novel β-Diketone type ligands having crown ether moiety, Kurahashi K, Umetani S, Yamazaki S, Ogura K, The 65th Conference on the Japan Society for Analytical Chemistry, 16 May 2004.

Distribution of trace metals in the Sulu Sea and the adjacent seas, Norisuye K, Ezoe M, Sohrin Y, The 51st

Annual Meeting of the Geochemical Society of Japan, 21 September 2004.

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.

In situ observations of dissolved Manganese in hydrothermal vent plumes at Mariana Trough, Okamura K, Yanai K, Sohrin Y, et al., American Geophisical Union 2004 Fall Meeting, 16 December 2004.

Grants

Sohrin Y, Interaction between metallome and proteome in the marine ecosystem, Grant-in-Aid for Scientific Research (A) (2), 1 April 2004 - 31 March 2007.

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

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°50'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).

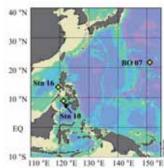


Figure 1. Location of stations (BO7 : the Northwest Pacific, Stn10 : the Sulu Sea, Stn16 : the South China Sea).

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.

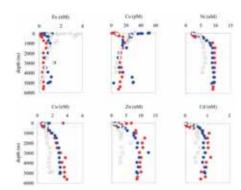


Figure 2. Vertical profiles of dissolved Fe, Co, Ni, Cu, Zn and Cd in the Sulu Sea (white circle), the South China Sea (blue circle) and Northwest Pacific (red circle).

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.

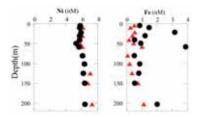


Figure 3. The distributions of dissolved and acid dissolvable Ni and Fe in upper water at 61°S (triangle: dissolved, circle: acid dissolvable).

Division of Environmental Chemistry - Solution and Interface Chemistry -

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The Hebrew University of Jerusalem, Israel, 9 - 10 March 2004

MOROOKA, Saiko (M2)

Universite Bordeaux I, France, 10 June 2004

CNRS, Universite Bordeaux I, France, 3 September 2004

Vis Prof of JSPS, University of Texas at Austin, USA, 4, 9 - 10 September 2004 President of AIRAPT (International Association for the Advancement of High Pressure

Science and Technology), Harvard University, USA, 13 September 2004

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.

Structure, Dynamics, and Reactions in Supercritical Water Studied by NMR and Computer Simulation, Nakahara M, The 14th International Conference on the Properties of Water and Steam, Kyoto, 30 August.

Development of a High-Temperature NMR Probe: Toward Temperature Homogeneity, Multinuclear Measurement, and High Magnetic Field Gradient, Nakahara M, Matubayasi N, Wakai C, and Yoshida K, The 14th International Conference on the Properties of Water and Steam, Kyoto, 2 September. Hydrothermal C1 Chemistry: Equilibrium Study,

Matubayasi N, Wakai C, Yoshida K, et al., The 14th International Conference on the Properties of Water and Steam, Kyoto, 2 September, and 39 related presentations.

Location and Side-Chain Conformation of a Neuropeptide, Achatin-I in Phospholipid Bilayer Membrane: A High-Resolution NMR Study, Kimura T, Okamura E, Matubayasi N, and Nakahara M, The Biophysical Society 48th Annual Meeting, USA, 18 February, and 2 related presentations.

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 (CO + $H_2O \rightleftharpoons CO_2 + H_2$) 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.

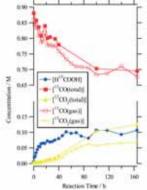


Figure 1. The time dependence of the product yields in the noncatalytic water-gas-shift reaction at 250°C.

Yoshida K, Wakai C, Matubayasi N, Nakahara M, J. Phys. Chem. A, 108, 7479-7482 (2004).

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.

Okamura E, Wakai C, Matubayasi N, Sugiura Y, Nakahara M, *Phys. Rev. Lett.*, **93**, 248101 (2004).

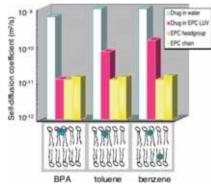


Figure 2. Mobility of drugs in membrane. In the upper graph are the self-diffusion rates of drugs in water (white) and in 100-nm vesicles (red) at 30°C, together with the mobility of membrane lipid head group (light yellow) and the chain core (yellow). Location of the drug in membrane is shown schematically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

April 2003 - 31 March 2006.

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

Nakahara M, Ion Transport Mechanism in Phospholipid Bilayer Membranes by Thermal Fluctuation, Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2005.

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

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

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

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

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.

Division of Environmental Chemistry- Molecular Microbial Science -

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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

Properties of an enzyme catalyzing the asymmetric reduction of 2-chloroacrylic acid, Kurata A, Kurihara T, Kamachi H, Esaki N, 2004 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 29 March.

Functional analysis of Suf proteins, Ano K, Kazuoka T, Mihara H, Kurihara T, Esaki N, 2004 Annual Meeting, Jpn. Soc. Biosci. Biotech. Agrochem., 29 March.

Identification of phosphorylated proteins by proteome analysis of a psychrotrophic bacterium, *Schewanella* sp. Ac10, Kawamoto J, Kurihara T, Kato T, Kitagawa M, Asada K, Kato I, Esaki N, 2004 Annual Meeting, Jpn. Biochem. Soc., 14 October.

Enzymatic synthesis of L-pipecolic acid by Δ^1 -piperideine-2-carboxylate reductase from *Pseudomonas putida*, Muramatsu H, Mihara H, Yasuda M, Ueda M, Kurihara

T, Esaki N, 2004 Annual Meeting, Jpn. Biochem. Soc., 14 October.

Grants

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

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

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

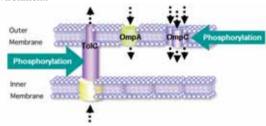


Figure 1. Membrane transport systems of *Shewanella* sp. Ac10 grown at 4° C.

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 hydroxypyruvate) 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-Lphenylalanine 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.

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

Kurihara T, Development of a low-temperature proteinproduction 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.

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

Award

KURIHARA T, 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, Jpn. Soc. Biosci. Biotech. Agrochem., 28 March 2004.

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

Research Activities (Year 2004)

Presentations

Thermal Expansion and Contraction of Polymer Thin Films, Kanaya T, Workshop on Auxetics and Related Systems, Poznan, Poland, 27 - 30 June (invited).

Reduced Viscosity of Linear and Spherical Polyelectrolyte Solutions: Differences and Similarities, Nishida K, Kanaya T, Kaji K, International Symposia on Polyelectrolytes, Massachusetts, 15 June.

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).

Structual Analysis of Drawing Polyethylene Blends with Ultra High Molecular Weight Component, Matsuba G, Ogino Y, Fukushima H, Kanaya T, Nishida K, 228th ACS National Meeting, Philadelphia, PA, USA, 24 August.

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.

Effect of Tacticity of Isotactic Polypropylene on Mesomorphic Phase Formation and Crystallization, Konishi T, Nishida K, Matsuba G, Kanaya T, Society of Polymer Science, Japan, Meeting, Soc. Polym. Sci, Hyogo, 25 May.

Dynamics of Polymer Thin Films in Picosecond Region as Studied by Inelastic and Quasielastic Neutron Scattering, Inoue R, Nishida K, Kanaya T, Tsukushi I, Shibata K, Autumn Meeting, Physical Society of Japan, Aomori, 12 September.

Effect of Ultra High Molecular Weight Component in Crystallization of Polyetylene under Shear Flow, Sakamoto S, Kanaya T, Nishida K, Matsuba G, 53th Symposium on Macromolecules, Hokkaido, September 16.

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 $Q_{\rm c}$, 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.



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

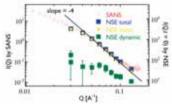


Figure 2. Scattering intensities of the first gel measured by SANS-U (+) and NSE (■) spectrometers. The intensity by NSE is divided into the static () and dynamic (■) fluctuations.

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

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

Kanaya T, Collaboratory on Electron Correlation Toward a New Research Network between Physics and

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 helixes 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 helixes 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.

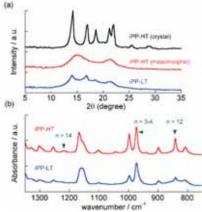


Figure 3. Wide angle X-ray diffraction profiles (a) and Fourier transform infrared spectra (b) of crystallized iPP-HT (black line), the quenched iPP-HT (red line) and the quenched iPP-LT (blue line). *n*: minimal number of 3/1 helical sequence.

Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2004 - 31 March 2006.

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

Division of Multidisciplinary Chemistry- Molecular Rheology -

http://molrheo.kuicr.kvoto-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, Microsymposium on Polymer Melt Rheology and Processing, Yonezawa, 17 - 18 March.

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.

Dynamic and Viscoelastic Study of Entanglement Dynamics, Watanabe H, II International Conference on Times of Polymers, Ischia, Italy, 20 - 23 June.

Nonlinear Rheology of Multiarm Star Chain and Related Soft Materials, Watanabe H, HUSC Conference - Colloids and Polymeric assemblies near to and far from equilibrium -, Crete, Greece, 25 - 27 June.

Dielectric and Viscoelastic Investigation of Entanglement Dynamics, Watanabe H, Polymer Physics Gordon

Conference, New London, USA, 1 - 6 August.

Viscoelastic and dielectric behavior of entangled blends of linear polyisoprenes: test of tube dilation 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.

Rheology of living bifunctional polybutadienyl dilithium chains in benzene: viscoelastic evaluation of aggregate lifetime, Oishi 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, Hirosaki, 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 Ap 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 ≥ 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.

1. H. Watanabe, Prog. Polym. Sci., 24(9), 1253-1403 (1999). 2. H. Watanabe and T. Inoue, Rheol. Acta, 43, 634-644 (2004).

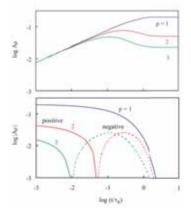


Figure 1. Evolution of anisotropies of Rouse eigenmodes during creep (top panel) and recovery (bottom panel). The anisotropy amplitudes are plotted against normalized time, t/τ_R ($\tau_R = \text{Rouse relaxation time}$).

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

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 $(N^+(CH_3)_4; TMA)$ 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 $\phi_{\text{TEA}} \ge 0.5$, the FOS threads/networks exhibited the Maxwell-type terminal relaxation reflecting their thermal scission. In this range of ϕ_{TEA} , the terminal relaxation time τ drastically increased with decreasing ϕ_{TEA} (see Figure 2.). On a further decrease of ϕ_{TEA} below 0.3, τ became insensitive to ϕ_{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 $\phi_{TEA} \ge 0.5$ 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).

- 1. H. Hoffmann and J. Würtz, J Molecular Liq, 72, 191 (1997). 2. H. Watanabe and T. Mori, J. Soc. Rheol. Japan, 32, 155-160 (2004). 3. H. Watanabe, T. Sato, K. Osaki, M. Matsumoto, D. P. Bossev, C. E.
- McNamee, and M. Nakahara, Rheol. Acta, 39, 110 (2000).

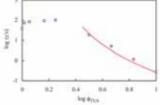


Figure 2. Dependence of terminal relaxation time of threadlike FOS micelles at 20°C on the TEA fraction in

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.kuicr.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 spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in mocrocapsules, boipolymers, 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.

A Study on Thin Films of Carrier-Doped Strontium Titanate with Taking Notice of Their Interfaces with Organic Thin Films, Sato N, Harada Y, Terashima T, Kanda R, Takano M, The 12th International Conference on Solid Films and Surfaces (Hamamatsu, Japan), 21 - 25 June.

Direct Observation of Electronic Structure of Unoccupied States in Metal Phthalocyanine Thin Films, Sato N, Yoshida H, Tsutsumi K, Third International Conference on Porphyrins and Phthalocyanines (New Orleans, USA), 11 -16 July.

Dielectric Behavior of a Microemulsion System Containing Water, Toluene and Triton X-100: Temperature dependent phase inversion, Asami K, 3rd International Conference on Broadband Dielectric Spectroscopy and its Applications, (Delft, The Netherlands), 23 - 26 August.

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.), Tamao K, Uchida M (Chisso 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

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

Yoshida H, Controlling Reactivity and Diffusion at 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 cupper 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.

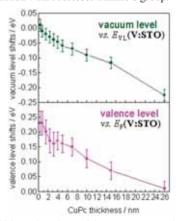


Figure 1. Thickness dependence of the apparent vacuum level and the valence level of CuPc overlayers on a V:STO film substrate. The upper panel: vacuum level with reference to that of V:STO, the lower panel: valence level with reference to its Fermi level.

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 maximums 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.

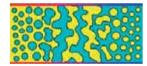


Figure 2. Temperature-dependent phase inversion of microemulsion.

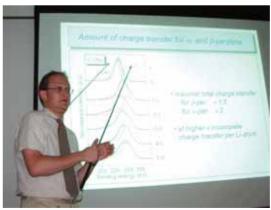


Figure 3. Dr. Rainer Friedlein from Linköping University, Sweden, gave a fascinating seminar.

Division of Multidisciplinary Chemistry - Supramolecular Biology -

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



Prof UMEDA, Masato (D Pharm Sc)



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



Assist Prof KATO, Utako (D Sc)



Res Associate INADOME, Hironori HAMASAKI, Maho (D Agr)



PD (ISPS) (D Sc)

Research Associates (pt)

YAMAGUCHI, Yukiko NISHIKAWA, Miwako

Students

TAKAHARA, Keigo (D1) TANIUCHI, Kentaro (M2)

Scope of Research

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

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

Research Activities (Year 2004)

Presentations

Transbilayer lipid movements: A role in cell division and cell polarity formation. Umeda, M. The 3rd Japanese Biochemical Society Biofrontier Symposium. New Aspect of Phospholipid Biology 2004. 10 - 12 May, Kamakura.

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.

Phylogenetic distribution of sphingomyelin in animals. Umeda, M. Aizu, M. Kobayashi, H. Gordon Research Conference, Glycolipid & Sphingolipid Biology, 25 - 30 July, Harima.

Role of ROS3 proteins, a regulator of membrane phospholipids organization, in cell morphogenesis. Kato U., Murata M., Umeda M. The 77th Annual Meeting of the Japaneese Biochemical Society. 13 - 16 October, Yokohama.

Removal of dystroglycan causes locomotor dysfunction

in Drosophila. Takeuchi K., Yamamoto D., Umeda M. The 77th Annual Meeting of the Japaneese Biochemical Society. 13 - 16 October, Yokohama.

Analysis of expression and function of Drosophila ROS3. Taniuchi K., Takeuchi K., Kato U., Umeda M. The 27th Annual Meeting of the Molecular Biology Society of Japan. 8 - 11 December, Kobe.

Grants

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

Umeda M, Identification of genes involved in thermoregulatory behavior of insects. Special Cooperation Funds for Promoting Science and Technology from the Ministry of Education, Sports, Science and Technology Agency of Japan. 1 April 2002 - 31 March 2005.

Takeuchi K, Development of a new Drosophila model for studying muscular dystrophy. Grant-in-Aid for Exploratory Research, 1 April 2004 - 31 March 2006.

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.

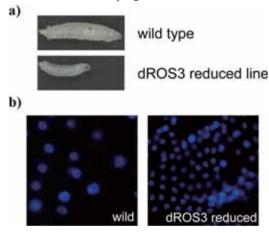


Figure 1. Suppression of dROS3 expression resulted in decreased cell and body sizes.

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.

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 $\Delta 9$ 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.

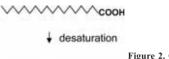


Figure 2. Oxidative desaturation of fatty acids by stearoyl-CoA desaturase.

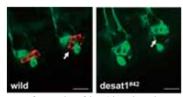


Figure 3. Patterns of expression of desat1 in embryonic oenocyte. Oenocyte (arrows) in wild type and the *desat1#42* mutant were immunostained with polyclonal antibodies raised against desat1 protein (red) and neuron-specific monoclonal antibody (green). Scale bars: 10 µm.

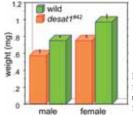


Figure 4. Body weight of male and female wild-type and the *desat1#42* mutant flies cultured on a fatty-acid-free defined medium.

Advanced Research Center for Beam Science - Particle Beam Science -

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



Prof NODA, Akira (D Sc)



Assoc Prof IWASHITA, Yoshihisa (D Sc)

2004



Assist Prof SHIRAI, Toshiyuki



Techn TONGU, Hiromu



PD TAKEUCHI, Takeshi (D Sc)

Lecturer (pt)

Prof Ogata, Atsushi (D Eng) Hiroshima University

Visitors

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Dr PARK, Seong Hee
Dr JEONG, Young Uk
Dr SIDORIN, Anatoly
Dr SMIRNOV, A
Prof LIN, Yuzhen
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Prof MESHKOV, Igor N.
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NAKAMURA, Shu (D3) FADIL, Hicham (D3) IKEGAMI, Masahiro (D3) YAMAZAKI, Atsushi (D2) FUJIMOTO, Shinji (D2) MIHARA, Takanori (D1) TANABE, Mikio (M2) ITOH, Hiroyuki (M1) SOUDA, Hikaru (M1)

Korea Atomic Energy Research Institute, Daejeon, Korea, 5 January 2004
Korea Atomic Energy Research Institute, Daejeon, Korea, 5 January 2004
Korea Atomic Energy Research Institute, Daejeon, Korea, 5 January 2004
Joint Institute for Nuclear Research (JINR), Dubna, Russia, 5 - 6 February 2004
Joint Institute for Nuclear Research (JINR), Dubna, Russia, 5 - 6 February 2004
Tsinghua University, Beijing, China, 17 March - 5 April 2004
Joint Institute for Nuclear Research (JINR), Dubna, Russia, 31 January - 6 March 2004
Joint Institute for Nuclear Research (JINR), Dubna, Russia, 18 - 26 April 2004
Max Planck Institute für Kemphysik, Heidelberg, Germany, 31 October - 12 November 2004
Lebedev Physical Institute, Russian Academy of Science, Moscow, Russia, 30 November

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

Laser Equipped Ion Storage and Cooler Ring, S-LSR, Noda A, Fadil H, Fujimoto S, Ikegami M, Iwashita Y, Nakamura S, Shirai T, Tanabe M, Tongu H, Matsukado K, Noda K, Shibuya S, Takeuchi T, Yamada S, Daido H, Kato Y, Tajima T, Beutelspacher M, Grieser M, Syresin E, Invited talk at the 3rd Asian Particle Accelerator Conference, Gyeongju, Korea, March 2004.

Laser Ion Production and its Medical Application, Noda A, Daido H, Fukumi A, Hashida M, Iwashita Y, Li Z, Matsukado K, Nakamura S, Sakabe S, Shimizu S, Shirai T, Tanabe M, Tongu H, Yamazaki A., Invited talk at Advanced Lasers and Their Applications, Jeju Island, Korea, May 2004.

Establishment of Advanced Research Center for Beam

Science, Institute for Chemical Research, Kyoto University-Aiming at creation of interdisciplinary research with use of the beam, Noda A, General Lecture at Autumn Meeting of Atomic Energy Society of Japan, Kyoto, September 2004.

Permanent Final Focus Magnet, Iwashita Y, Mihara T, Kumada M, Sugiyama E, International Conference on Linear Colliders, 21 April 2004.

Velocity compliant bunching with amplitude modulation, Iwashita Y, 6th International Workshop on Neutrino Factories & Superbeams, 27 July 2004.

A Super-Strong Permanent Magnet Quadrupole with Variable Strength, Iwashita Y, Mihara T, Evgeny A, Kumada M, Spencer C.M, Sugiyama E, XXII International Linear Accelerator Conference, Lübeck, 17 August 2004.

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 $\pm 1\%$ 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 is 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.

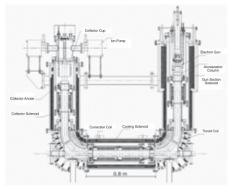


Figure 1. Cross-sectional view of the electron cooler for S-LSR.



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

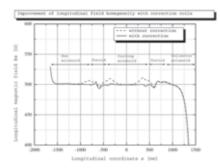


Figure 3. Improvement of the uniformity of the longitudinal field strength along the electron orbit with use of the correction coils attached at the transient regions between solenoids and troids.

Adjustable Strong Permanent Magnet for Final Focus Quadrupole, Mihara T, Iwashita Y, Kumada M, Spencer CM, The 7th ACFA workshop on Physics & Detector at the Linear Collider, 11 November 2004.

Final Doublet, Mihara T, Napoly O, First ILC Workshop, 14 November 2004.

Grants

Noda A, Beam Accumulation and Cooler Ring, Ad-

vanced Compact Accelerator Research, April 2001 - March 2006.

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

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

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

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



Prof SAKABE, Shuji (D Eng)



Assist Prof HASHIDA, Masaki (D Eng)



Assist Prof SHIMIZU, Seiji (D Sc)

Students KAGAWA, Takeshi (D2) SHIRAI, Kouta (M1)

Visitor

Prof NICLES, Peter Max-Born-Institute, Germany, 17 June 2004

Scope of Research

The research subjects are ultra-intense and ultra-short laser-matter interactions and their applications. The physics of nano-ablation 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 radiation 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 chemistry, biology, material physics, 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.

Research Activities (Year 2004)

Presentations

Ion generation in a low density plastic foam by Coulomb explosion with an intense femtosecond laser", S. Sakabe, M. Hashida, S. Shimizu, T. Iida, F. Sato, S. Okihara, K. Nishihara, T. Zh. Esrkepov, T. Norimatsu, K. Nagai, and Y. Izawa, International Workshop on Fast Ignition and High Field Physics 2004, 25 - 29 April 2004, Kyoto, Japan.

Proton generation from hydrogen cluster Coulombexploded by intense femtosecond laser pulses, M. Hashida, S. Sakabe, S. Shimizu, T. Iida, F. Sato, S. Okihara, T. Kagawa, K. Nishihara, K. Imasaki, and Y. Izaw, International Workshop on Fast Ignition and High Field Physics 2004, 25 - 29 April 2004, Kyoto, Japan.

Coulomb-explosion of argon cluster intense femtosecond laser pulses, S. Shimizu, S. Sakabe, M. Hashida, T. Iida, F. Sato, S. Okihara, M. Hirokane, T. Kagawa, and Y. Izawa, International Workshop on Fast Ignition and High Field Physics 2004, 25 - 29 April 2004, Kyoto, Japan.

Possibilities of controllable ablation by femtosecond lasers, A. Kinoshita, M. Fujita, M. Hashida, Y. Izawa, T. Nakayama, M. Katto, and K. Nagashima, LPM2004 20 - 21 May 2004, Nara-ken New public hall, Japan.

X-ray spectroscopic measurements to study energy transport by hot electrons in ultra-intensity laser produced

plasma, H. Nishimura, Y. Inubushi, M. Ochiai, S. Fujioka, T. Kawamura, S. Okihara, M. Hashida, S. Simizu, S. Sakabe, S. Kato, F. Koike, S. Nakazaki, T. Matsuoka, R. Kodama, K. A. Tanaka, K. Mima, H. Nagatomo, T. Johzaki, Y. Kitagawa, H. Fujita, T. Jitsuno, N. Miyanaga, T. Norimartsu, K. Nagai, and Y. Izawa, International Symposium on Ultrafast Intense Laser Science 3, September 16 - 20, 2004, Palermo, Sicily.

Grants

Sakabe S, Fundamental Research on γ-ray Laser with Intense Femtosecond Lasers, Grant-in-Aid for Scientific Research (B)(2), 1 April 2003 - 31 March 2005.

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

Award

Hashida M, Furukawa H, Tsukamoto M, Fujita M, Izawa Y, 2003 LSJ Award for Distinguished Achievements in research, Femtosecond laser ablation of metals: characterization of new processing region and formation of nanostructures The Laser Society of Japan, 28 May 2004.

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, Kvoto 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 chirpedpulse 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

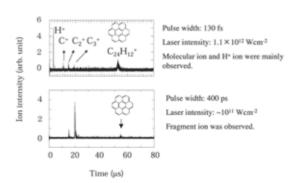
Energy distributions of ions emitted from argon clusters (up to 12 800 atoms/ cluster) Coulomb-exploded with an intense femtosecond laser have been experimentally studied. Under the laser intensity of $2x10^{16}$ W/cm², the ions of >15 keV are anisotropically emitted, while those lower than 15 keV tend 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^{8+} - Ar^{14+} ions depend on laser polarization direction, while those of Ar^{4-} Ar⁷⁺ 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/cm² for copper. The spacing d of the patterned structure was determined to be $d = 300\pm40$ nm for 0.07 J/cm² and d = 600±40 nm for 0.22 J/cm². 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 siganl 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 possiblility as a new soft-ionization method.



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

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



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Assist Prof OGAWA, Tetsuya (D Sc)



Assist Prof (D Sc)



Res Associate NEMOTO, Takashi MORIGUCHI, Sakumi (D Sc)



YOSHIDA, Kaname KOSHINO, Masanori (D Sc)



Res



PD YAJI, Toyonari (D Sc)

Students

KUWAMOTO, Kiyoshi (RF) TSUJIMOTO, Masahiko (RF) TAKAJO, Daisuke (D3) MINARI, Takeo (D2) MIYAMOTO, Yusuke (D2) KIYOMURA, Tsutomu (M2) KUBOTA, Yuzuru (M2) HARUTA, Mitsutaka (M1) NAGAMATSU, Daiki (M1)

Visitors

Prof YUAN, J Tsinghua University, China, 12 June 2004

Dr MAGONOV, S Digital Instruments/Veeco Metrology, USA, 14 June 2004

Prof MILES, M, J H.H.Wills Physics Laboratory, University of Bristol, UK, 2 July 2004

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

Cryo-TEM Observation of the Formation Process of Gold Nano-rod in an Aqueous Solution of Surfactant, Ogawa T, Kurata H, Isoda S, International Symposium on the Creation of Novel Nanomaterials, 20 January.

Core Hole Effects on the Oxygen K-ELNES of Transition Metal Oxides, Kurata H, Tsujimoto M, Nemoto T, Isoda S, 8th APEM, 7 June.

Nano-scale 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-benzoquinonedioximato) Platinum(II), Yoshida K, Yaji T, Isoda S, EM-NANO 2004, 8 June.

Transport Properties of Single-grain Organic Fieldeffect Transistor, Minari T, Nemoto T, Isoda S, The International Symposium on Super-Functionality Organic Devices, 26 - 28 October.

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., JJAP, 43(7B), 4667 (2004).

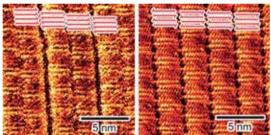


Figure 1. STM images of the α - and β -form stearic acid on HOPG.

$DV-X_{CA}$ Calculation of Electron Energy-Loss Near-Edge Structures of F₄TCNQ

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-quinodi-

methane (F4TCNQ) and 7,7,8,8-tetracyanoquinodimethane (TCNQ). Electron energy-loss spectra (EELS) of F4TCNQ were measured and analyzed through the calculation. In the discrete variational- $X\alpha(DV-X\alpha)$ 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 F4TCNO, 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 fluorination effect on the quinoid-ring carbons appearing in the higher σ^* energy region. In the low energy region, the calculations accurately reproduced the coreexcited spectra in both F4TCNQ and TCNQ and succeeded in assigning each component appearing in the spectra.

Koshino M et al., J. Electron Spectroscopy & Related Phenomena, 135(2-3), 191, (2004).



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

Nanodiffraction and Characterization of Titanate Nanotube Prepared by Hydrothermal Method, Kubota Y, Kurata H, Isoda S, Korea-Japan Joint Forum 2004, 3 - 6 November.

First Principles Calculations of Electron Energy-Loss Near-Edge Structure of Transition Metal Compounds, Kurata H, Tsujimoto M, Nemoto T, Isoda S, IUMRS International Conference in Asia, 15 - 17 November.

Grants

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004 - 31 March 2005.

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

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

Kurata H, Development of an EELS/XES Electron Microscope for Electronic Structure Analysis, Leading Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004 - 31 March 2006.

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 spectromator with a high-resolution in order to elucidate the property of materials. The theoretical analysis of the electronic states with DV- $X\alpha$ 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

X-Ray Crystal Structure Analysis of the Complex between Carboxypeptidase Y and a Protein Inhibitor I^C, Mima J (Kyoto University), Hayashida M, Fujii T *et al.*, Annual Meeting, Jpn Soc. Biosci. Biotech. Agrochem., 29 March.

Crystallization and Preliminary X-ray Analysis of Carboxypeptidase Y Inhibitor I^C Complexed with the Cognate Proteinase, Mima J (Kyoto University), Hayashida M, Fujii T *et al.*, Acta Crystallogr. **D60**, 1622 - 1624 (2004).

X-Ray Crystal Structure Analysis of a Complex between Carboxypeptidase Y and a Protein Inhibitor, Hata Y, Hayashida M, Fujii T *et al.*, 6th Conference, Asian Crystallogr. Assoc., 28 June.

Crystal Structure of a Protein Complex and Functional Analysis of Mutants of Multi-functional Protease Inhibitor I^C with Phospholipid Binding Activity, Mima J (Kyoto University), Hayashida M, Fujii T *et al.*, Annual Meeting, Mol. Biol. Soc. Jpn, 9 December.

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 pyroelectric 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 Feburary (invited).

Grants

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

Sanjoh A (Protein Wave Corporation), Hata Y *et al.*, Studies and Developments on Practical Use of Devices for Growth of Protein Crystals Suitable for Ultra-high Resolution X-ray Analysis, Grant for Spport of Studies and Developments by Cooperation of Industry, Academic and Public, Kyoto Sangyo 21 Foundation, 1 April 2004 - 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. C^{α} -deviation over five consecutive residues after C^{α} -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.

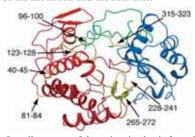


Figure 1. Overall structure of the active site that is formed by three subunits, A-, B-, and C-chains, which are colored green, blue, and red, respectively. Structurally different regions are colored yellow.

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

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

We have made a structural model of the complex in which a substrate L-aspartate was manually docked into the active site of *Bacillus* sp. YM55-1 aspartase as followings (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 –NH₃⁺ 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, Lys324 is only one positively charged residue in the activesite 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 Lys324 and Ser140 with the dipole moment of α -helix, respectively.

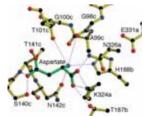


Figure 2. The putative binding mode of substrate L-aspartate in the active site. The docked model of the substrate is represented by green bonds. Putative hydrogen bonds are shown by broken lines.

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

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 σ -conjugation in the polysilane framework using the configuration-constrained oligosilane model systems, (2) development of intramolecular electron transfer systems through σ -conjugated oligosilane chains, (3) construction and application of new polycyclic systems including main group elements, (4) development of new efficient reactions using main group element reagents and transition metal complex catalysts, and (5) design and synthesis of novel π -conjugated systems containing main group elements.

Research Activities (Year 2004)

Presentations

My Favorite Silicon and Boron (invited), Tamao K, Herbert C. Brown Lecture, 3 April, Purdue University,

Sigma-Conjugated Oligosilanes – Conformation Dependence of the Photophysical Properties (invited), Tamao K, Tsuji H, 17th IUPAC Conference on Physical Organic Chemistry (ICPOC17), 15 - 20 August, Shanghai, China.

Palladium-Catalyzed Cross-Coupling Reaction of Aryltriazene with Organometallic Reagents, Saeki T, Son E-C, Matsunaga T, Tamao K, 51st Symposium on Organometallic Chemistry, 22 October, Tokyo, Japan.

Elemento-Organic Chemistry Directed toward Materials Science, Tamao K, The First International Symposium on Functional Innovation of Molecular Informatics (invited), 13 - 15 October, Kyushu University, Fukuoka, Japan.

Elemento-Organic Chemistry Directed toward Materials Science, Tamao K, The 2nd International Symposium of the 21COE Program, Center for Practical Nano-Chemistry, 21 - 22 December, Waseda University, Tokyo, Japan.

Grants

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

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.

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

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 conformation dependence of the oligosilane σ conjugation: the *anti* conformation (SiSiSiSi dihedral angle $\omega=180^\circ$) 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 $\sigma\sigma^*$ transition is much narrower even at room temperature as compared with $n\text{-Si}_5\text{Me}_{12}$. 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.

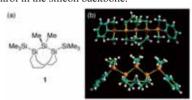


Figure 1. (a) Structure of all-anti pentasilane 1. (b) X-ray structure of the *all-anti* pentasilane derivative.

Reference: Tsuji H, Fukazawa A, Yamaguchi S, Toshimitsu A, Tamao K *Organometallics* **2004**, 23, 3375-3377.

Cross-Coupling Reaction of 1-Aryltriazenes with Organotrifluorosilanes

We have recently reported that the cross-coupling reaction of 1-aryltriazenes with areneboronic acids readily pro-

ceeds 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 carbonnitrogen bond to the zero-valent palladium complex.

$$Ar-N$$

Pd catalyst, PR_3 ,
 $BF_3 \cdot OEt_2$
 $Ar-Ar'$
 $DME. rt$
 $Ar-Ar'$

Scheme 1. Cross-coupling reaction of 1-aryltriazenes with areneboronic 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. Cross-coupling reaction of 1-aryltriazene with aryltrifluorosilane (plausible reaction mechanism)

The reaction system is applicable to the cross-coupling reaction with alkenyl-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. Cross-coupling reaction of 1-(p-tolyl)triazene with (E)-styryltrifluorosilane.

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

[1] T. Saeki, E.-C. Son, K. Tamao, *Org. Lett,* **2004**, 6, 617., [2] T. Saeki, T. Matsunaga, E.-C. Son, K. Tamao, *Adv. Synth. Catal.* **2004**, 346, 1689.

Control of Conformation and Photophysical Properties of Oligosilanes Based on Bicyclic Structure, The Society of Silicon Chemistry, Japan, 29 October.

Tsuji H, The ICR Award for Young Scientists, Conformation Control of Oligosilanes Based on Bicyclic Structure, ICR, 3 December.

Fukazawa A, Best Poster Award for Graduate Students, ICR, Conformation Control of Oligosilanes Based on Bicyclic Trisilane Unit, ICR, 5 March.

Fukazawa A, Symposium Poster Award, 51th Symposium on Organometallic Chemistry, Japan, 15 December.

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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 $T_{\rm C}$ Superconductor Kan 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), SaitoT, Azuma M, Kanda H, Takano M, et al., 4th International Conference on Inorganic Materials,19 - 21 September (Antwerp).

Current-induced first-order transition in the microfabricated perovskite manganese oxide thin films, Masuno A, Terashima T, Mikio T, 60th Annual Meeting, The Physical Society of Japan, 12 - 15 September (Aomori).

Synthesis, physical properties of Ca_{2-x}CuO₂Cl₂, Yamada I, Azuma M, Shimakawa Y, Takano M, 60th Annual Meet-

ing, The Physical Society of Japan, 12 - 15 September (Aomori).

Light emission from oxygen deficient SrTiO₃, 93rd Annual Meeting, Japan Society of Powder and Powder Metallurgy, Kanda R, Kan D, Masuno A, Terashima T, Takano M, 25 - 27 May (Kyoto).

Grants

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

Terashima T, Electric field induced superconductivity in the FET devices using ultrathin SrTiO₃ single-crystal substrate with high dielectric constant, Grant-in-Aid for Scientific Research (B) (2), 1 April 2002 - 31 March 2004.

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

We have found a novel cobalt oxide, SrCo₆O₁₁, by high pressure synthesis technique. As shown in figure 1, SrCo₆O₁₁ comprises Co₃O₈ Kagome layers with CoO₆ octahedra and CoO₅ 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.

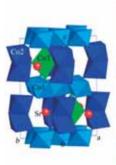




Figure 1.Crystal structure of SrCo₆O₁₁ and the high pressure synthesis apparatus.

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

New type of heterojunctions comprising of YBa₂Cu₃O_{7-δ} (YBCO; p-type) and oxygen-deficient SrTiO₃ (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.

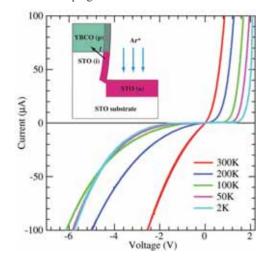


Figure 2. I-V characteristics for YBCO/STO p-i-n junction.

Synthesis of Monodisperse, Submicron-Sized Spherical V₂O₅ 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 V₂O₅ 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. V₂O₅ particles are possibly used in catalysis, lithium ion battery, electrochromic device, sensors and actuators. The monodisperse spherical V₂O₅ particles obtained by our developed method will greatly improve the performance in such applications.

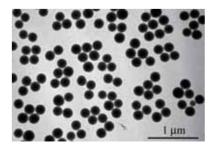


Figure 3. Transmission electron microscope image of V_2O_5 particles.

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Scope of Research

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

Highly Selective Ring-Opening Cross-Metathesis Reactions Using Fischer-type Carbene Ruthenium Catalysts, Katayama H, Fukuse Y, Nagao M, Ozawa F, The 3rd International Symposium of the Kyoto COE Project "Elements Science", 9 - 10 January, Kyoto, Japan.

Catalytic C-O Bond Cleavage of Allylic Alcohols Using Diphosphinidenecyclobutene-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.

Facile and Selective Deallylation of Allyl Ethers Using Diphosphinidenecyclobutene-Coordinated Palladium Catalysts, Ozawa F, Murakami H, The 12th Japan-Korea Joint Symposium on Organometallic and Coordination Chemistry, 3 - 6 August, Sendai, Japan.

Bromination of Four Acetylenic Protons Cp'4Fe4(HCCH)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.

Fischer-type Ruthenium Carbene Complexes: Highly Selective Catalysts for Ring-Opening/Cross Metathesis, Nagao M, The 2nd Trilateral Workshop on Organic Chemistry, 4 - 6 September, Kyoto, Japan.

Reaction Chemistry of Platinum-Group 14 Element Bonds, Ozawa F, JSCC Symposium 2004, 23 - 25 September, Kumamoto, Japan.

Stereocontrolled Synthesis and Photochemistry of cis-Poly(arylene vinylene)s, Katayama H, Nagao M, Nishimura T, Matsui Y, Akamatsu K (Konan Univ.), Nawafune H (Konan Univ.), Ozawa F, 50th Symposium of Organometallic Chemistry, Japan, 22 - 23 October, Tokyo, Japan.

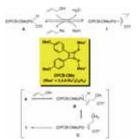
Grants

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

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

We recently found that $(\pi$ -allyl)palladium complex 1 bearing 1,2-bis(4-methoxyphenyl)-3,4-bis(2,4,6-tri-tertbutylphenylphosphinidene)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 \mathbb{C} , forms π -allyl complex 1. We reasoned that strong π -accepting ability of DPCB-OMe ligand as an sp²-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.



Scheme 1. Direct conversion of allylic alcohol catalyzed by (DPCB-OMe)Pd(π -allyl) complex 1.



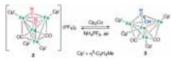
Scheme 2. Deallylation of allyl ethers catalyzed by 1.

- 1. Ozawa, F.; Ishiyama, T.; Yamamoto, S.; Kawagishi, S.; Murakami, H.; Yoshifuji, M. *Organometallics* **2004**, 23, 1698.
- 2. Murakami, H.; Minami, T.; Ozawa, F. J. Org. Chem. 2004, 69, 4482.

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

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

Two-electron reduction of 2 resulted in the coupling of two methylidyne 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 methylidyne fragments via two-electron oxidation and reduction.

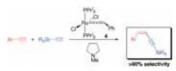


Scheme 3. Reversible carbon-carbon bond formation induced by two-electron redox reaction.

3. Okazaki, M.; Ohtani, T.; Ogino, H. J. Am. Chem. Soc. 2004, 126, 4104.

(Z)-Selective Cross-Dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinylideneruthenium 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 K_2CO_3 in MeOH to give terminal alkenylacetylenes (ArCH=CH-C \equiv CH) with (Z)-configurations.



Scheme 4. Ruthenium-catalyzed cross-dimerization between arylacetylenes and silylacetylenes.

Award

Ozawa F, The BCSJ Award, Insertion of Phenylacetylene into [Pt(GeMe₃)(SnMe₃)(PMe₂Ph)₂], The Chemical Society of Japan, 15 July 2004.

International Research Center for Elements Science - Photonic Elements Science -

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



Prof KANEMITSU, Yoshihiko MATSUDA, Kazunari (D Eng)



Assoc Prof (D Eng)



Assist Prof INOUYE, Hideyuki (D Eng)

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.

Luminescence Properties of Single Semiconductor Nanoparticles Embedded in Transparent Films (invited), Kanemitsu Y, 2004 International Symposium on Organic and Inorganic Electronic Materials and Related Nanotechnologies, 7 - 10 June, Niigata, Japan.

Optical Properties of Wide Band-Gap Semiconductors (invited), Kanemitsu Y, The 65th Autumn Meeting, The Japan Society of Applied Physics, 1 - 4 September, Sendai, Japan.

Photoluminescence Dynamics of Highly Excited GaN (invited), Nagai T and Kanemitsu Y, The 65th Autumn Meeting, The Japan Society of Applied Physics, 1 - 4 September, Sendai, Japan.

Advanced Nano-scale Optical Spectroscopy of Semiconductor Quantum Structures (invited), Matsuda K, The 1st International Symposium on Synchrotron Radiation Nanomaterials Science and Technology, 15 - 17 March, Tokyo, Japan.

Near-field Optical Mapping of Exciton and Biexciton Wavefunctions Confined in a Semiconductor Quantum Dot (invited), Matsuda K, The Conference on Lasers and Electro-Optics/International Quantum Electronics Conference, 16 - 21 May, San Francisco, USA.

Real-space Mapping of Exciton Wave Function in a GaAs Quantum Dot by Near-field Imaging Spectroscopy (invited), Matsuda K, 6th International Conference on Excitonic Processes in Condensed Matter, 6 - 9 July, Cracow, Poland.

Imaging Spectroscopy of Semiconductor Quantum Structures by Near-field Scanning Optical Microscope with a High Spatial Resolution (invited), Matsuda K, 2004 Autumn Meeting, The Physical Society of Japan, 12 - 15 September, Aomori, Japan.

Nano-imaging Spectroscopy of Semiconductor Quantum Structures (invited), Matsuda K, The 4th NSF-MEXT Joint Symposium on Nano-photonics, 27 - 29 October, Tokyo, Japan.

Grants

Kanemitsu Y, Fabrication of Impurity-doped Semiconductor Nanoparticles and Optical Responses of Single Semiconductor Nanoparticles, Grant-in-Aid for Scientific Research (B)(2), 1 April 2002 - 31 March 2005.

Matsuda K, Wavefunction Imaging and Control in Semiconductor Nano-structure by Ultimate Optical Nanoprobe, Precursory Research for Embryonic Science and Technology, Japan Science and Technology Agency, 1 November 2002 - 31 October 2005.

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.

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 Kerrgate time-resolved photoluminescence measurements (Fig. 1).

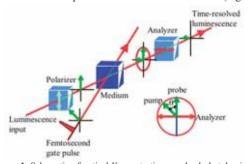


Figure 1. Schematic of optical Kerr-gate time-resolved photoluminescence measurements using femtosecond laser pulses.

Optical Near-field Spectroscopy of Semiconductor Quantum Structures

Scanning near-field optical microscope with a spatial resolution of 100-150 nm ($\lambda/7$ - $\lambda/5$, λ : wavelength of light) has contributed to explorer 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-excitons 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.

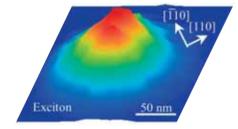


Figure 2. Exciton wave function image in a GaAs quantum dot by near-field photoluminescence mapping.

Awards

Kanemitsu Y, Phosphor Award, Pioneering Contributions for Semiconductor Nanoparticles, Phosphor Research Society, The Electrochemical Society of Japan, 26 November 2004.

Matsuda K, Research Award, Near-field Optical Mapping of Exciton Wave Function in a GaAs Quantum Dot, Research Foundation for Opto-Science and Technology, 16 March 2004.

Inouye H, Best Young Presenter Award, Ultrafast Response of a Self-organized Closely-packed Metal Nanoparticles System, Society of Nano Science and Technology, 10 May 2004.

Bioinformatics Center - Bioknowledge Systems -

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



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Scope of Research

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

Research Activities (Year 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).

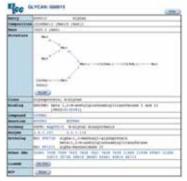


Figure 1. Structure based glycan database, KEGG GLYCAN.

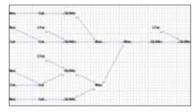


Figure 2. Extracted characteristic glycan structure of mouse.

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 PATH-WAY 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.

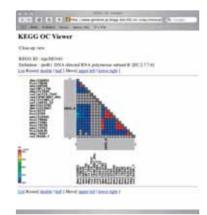


Figure 3. Ortholog Cluster Viewer on KEGG SSDB.

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.

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

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

Bioinformatics Center - Biological Information Network -

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



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Visitors

Mr FENG, Eric Prof NG, Michael Kwak-Po Dr CHING, Wai Ki

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, scalefree networks, protein structure prediction, inference of biological networks, chemo-informatics, discrete and stochastic methods for bioinformatics.

Research Activities (Year 2004)

Presentations

Fast algorithms for comparison of similar unordered trees, Fukagawa D, Akutsu T, The 15th Annual Int'l Symp. on Algorithms and Computation, 21 December.

Algorithms for point set matching with k-differences, Akutsu T, The 10th Int'l Computing and Combinatorics Conference, 18 August.

Extensions of marginalized graph kernels, Mahé P, Ueda N, Akutsu T, Perret J-L and Vert J-P, The 21st Int'l Conf. on Machine Learning, 4 July.

A simple method for inferring strengths of protein-protein interactions, Hayashida M, Ueda N, Akutsu T, The 4th Int'l Workshop on Bioinformatics and Systems Biology, 2 June.

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

Protein threading with profiles and constraints, Akutsu T, Hayashida M, Tomita E, Suzuki J, Horimoto K, IEEE 4th Symp. on Bioinformatics and Bioengineering, 21 May.

Protein side-chain packing problem: a maximum edgeweight clique algorithmic approach, K.C. D., Akutsu T, Tomita E, Seki T, The 2nd Asia-Pacific Bioinformatics Conference, 20 January.

Grants

Akutsu T, Miyano S, Maruyama O, Ueda N, Algorithms for extracting common patterns from structured biological data, Grant-in-Aid for Scientific Research (B), 1 April 2004 - 31 March 2008.

Akutsu T, Genome information science (a member of the project), Grant-in-Aid for Scientific Research Proiority 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^{-r} , where r is a constant. Such a network is called a scale-free network with exponent -r, 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 -r; its transformed network L(G) is also a scale-free network with exponent -r+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.

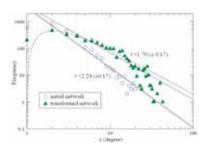


Figure 1. The distribution of the degree of nodes in the initial metabolic network from the KEGG database and its transformed networks.

Nacher J C, Yamada T, Goto S, Kanehisa M, Akutsu T, Two complementary representation of a scale-free network, *Physica A*, in press (2004).

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.

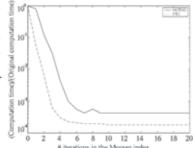


Figure 2. Computation time using different number of iterations of the Morgan index for the MUTAG and PTC data sets.

Mahé P, Ueda N, Akutsu T, Perret J-L, Vert J-P: Extensions of marginalized graph kernels, *Proc. 21st Int'l Conf. on Machine Learning*, 552-559 (2004).

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.

Contributed Chair - Proteome Informatics (SGI Japan) -

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



Vis Assoc Prof MAMITSUKA, Hiroshi YAMAGUCHI, Atsuko (DSc)



Vis Assist Prof (D Inf)



Vis Assist Prof AOKI, Kiyoko F. (PhD)



PD WAN, Raymond (Ph D)



PD ZHU, Shanfeng (Ph D)

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

A General Probabilistic Framework for Mining Labeled Ordered Trees, Ueda, N, Aoki, K F, Mamitsuka, H, Fourth SIAM International Conference on Data Mining (SDM 2004), Orlando, FL, USA, 23 April.

Application of Machine Learning to Bioinformatics, Mamitsuka H, Summer School of Bioinformatics (Sponcered 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.

A Hierarchical Mixture of Markov Models for Finding Biologically Active Metabolic Paths using Gene Expression and Protein Classes, Mamitsuka H, 2004 IEEE

Computational Systems Bioinformatics Conference (CSB 2004), Stanford, CA, USA, 19 August.

Glycan Tree Alignment and Substitution Matrix for Finding Relationships between Glycan Linkages, Aoki K F, US/Japan Glyco 2004 (Joint Meeting of the Society for Glycobiology and the Japanese Society of Carbohydrate Research), Honolulu, HI, USA, 20 November.

Analyzing Metabolic Pathways using Expression Profiles, Mamitsuka H, Workshop, 27th Annual National Meeting of the Molecular Biology Society of Japan, Kobe, Japan, 9 December.

Grant

Mamitsuka, H., Developing Algorithms for Searching and Finding Small Chemical Compounds Binding to Large Biological Molecules, Grant-in-Aid for Scientific Research on Priority Areas (C), 1 April 2004 - 31 March 2005.

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.

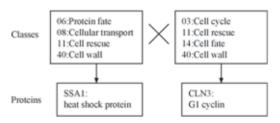


Figure 1. Example of two interacting proteins and the latent knowledge (protein classes).

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 lableled unordered trees, we have

Monosaccharide name	Abbr.	Sym.
Glucose	Gle	•
Galactose	Gal	•
Mannose	Man	0
N-acetyl neuraminic or sialic acid	NeuNAc	•
N-acetylglucosamine	GlcNAc	
N-acetylgalactosamine	GalNAc	
Fucose	Fuc	
Xylose	Xyl	∇
Glucuronic acid	GlcA	٠
Iduronic acid	IdA	÷

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

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.

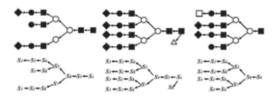


Figure 3. Example of multiple tree alignment obtained by the proposed probabilistic model.

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Assoc Prof KUMA, Keiichi (D Sc)



Assist Prof DAIYASU Hiromi (D Sc)



Assist Prof ICHIHARA Hisako



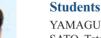
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PD HOSHIYAMA, Daisuke (D Sc)



PD YOKOI, Toshiro (D Agr)



YAMAGUCHI, Takeshi (D5) SATO, Tetsuya (D1)

NEMOTO, Wataru (D2)

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.

Evolutionary analysis of membrane-associated proteins, Toh H, Ichihara H, Daiyasu H, 1st Pacific-Rim International Conference on Protein Science, 16 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.

MAFFT: a multiple sequence alignment program, Katoh K, Misawa K (Kazusa DNA Research Institute), Kuma K, Toh H, Miyata T (JT Biohistory Research Hall, Waseda University), 76th Annual Meeting of the Genetics Society of Japan, 28 September. Molecular evolution of polar lipid biosynthesis in Archaea, Toh H, Yokoi T, Daiyasu H, 27th The Molecular Biology Society of Japan, 8 December.

Computational Analysis of Substrate Specificity of Disaccharide-Specific Glycosidase, Daiyasu H, Mizutani M, Sakata K, Toh H, 27th The Molecular Biology Society of Japan, 9 December.

Optimized MAFFT: improvement in accuracy of multiple sequence alignment, Katoh K, Kuma K, Toh H, Miyata T (JT Biohistory Research Hall, Waseda University), 27th Annual Meeting of the Molecular Biology Society of Japan, 9 December.

Database for GPCRs Interaction Partners -GRIP-, Nemoto W, Toh H, 27th The Molecular Biology Society of Japan, 9 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 DNAcoded 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, teleost 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 teleost 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.

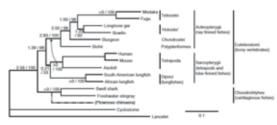


Figure 1. The maximum likelihood tree inferred from the concatenated amino acid sequences (2,942 residues) of seven proteins.

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, Kanehisa M, Toh H, 15th International Conference on Genome Informatics, 13-14 December.

Grants

Toh H, Development of the tools for protein structure comparison, BIRD, 1 April 2004 - 31 March 2005.

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 zebrafish 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 sub family. This is the first report of the CRY-DASH members from vertebrates and fungi.

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

Toh H, Domain Prediction in Structural Genomics for

Toh H, Domain Prediction in Structural Genomics for Signal Transduction (Inagaki group), Protein 3000, 1 April 2004 - 31 March 2005.

Toh H, Development of the Computational method to analyze soft protein-protein interactions, Grant-in-Aid for Scientific Research, 1 April 2004 - 31 March 2005.

Award

Toh H, The Okawa Publications prize, Bioinformatics for the Analysis of Protein Function, The Okawa Foundation, 25 November.

VISITING PROFESSORS' ACTIVITIES IN ICR



Vis Prof TAKAHASHI, Hideroh (D Eng)

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
- 5) Development of Meso-Porous Materials II -Synthesis of Meso-Porous Organic Silica-



Vis Prof KYOTO, Michihisa (D Eng)

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.



Vis Prof KITAZAWA, Koichi (Ph D)

Laboratory of Advanced Solid State Chemistry

Executive Director, Japan Science and Technology Agency (4-1-8 Honmachi, Kawaguchi, Saitama 332-0012)



Vis Prof NAGASAWA, Koichi (D Sc)

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 YAN, Chun-hua (Ph D)

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 Assoc Prof SAITO, Susumu (D Eng)

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



Vis Assoc Prof TSUKAGOSHI, Kazuhito (D Sc)

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



Vis Assoc Prof EMOTO, Kazuo (D Pharm Sc)

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



Vis Assoc Prof MATSUMOTO, Yonetatsu (D Eng)

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

Personal

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 metallobiochemistry 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 bioinorganic 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 enediyne antitumor antibiotics known by their strong antitumor activities. He firstly clarified the sequence- or conformation-specific DNA cleavage manners by endiyne antitumor antibiotics including esperamicin, dynemicin, C-1027, and

so on. For the recent years he investigated the mechanism of DNA recognition of the Cys2His2-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-fu 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 Mitsui 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 miceller 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-CCl4 interface by resonance Raman spectroscopy. He found that in certain basic pH's, the tautomeric structural change from the azo form to the protonated hydrazone 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 hyper-

coordinate 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 σ -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 C_{60} " 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 Govenor's Award

Outstanding Leader in High Pressure Gas Production Safety Manager

26 October 2004

SAITO, Shigeki



The ICR Award for Students

"Arabidopsis CYP707As Encode (+)-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

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

KANEMITSU, Yoshihiko



Phosphor Award

"Pioneering Contributions for Semiconductor Nanoparticles"

Phosphor Research Society, The Electrochemical Society of Japan

26 November 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

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

INOUYE, 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

TOH, 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 Sciences, Kyoto University, ⁴ International Institute for Advanced Studies



OZAWA, Fumiyuki, et al.

The BCSJ Award

"Insertion of Phenylacetylene into [Pt(GeMe₃)(SnMe₃)(PMe₂Ph)₂]" 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

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

INOUE, Rintaro



The Best Poster Award

UK-Japan Polymer Workshop

"Inelastic Neutron Scattering from Polystyrene Thin Films"

UK-Japan Polymer Workshop

1 April 2004

MAEDA, Shuhei



The Best Poster Award

The 17th Symposium on Fundamental Organic Chemistry

"Encapsulation of Molecular Hydrogen into an Open-Cage Fullerene C₇₀ Derivative"

The Committee of the 17th Symposium on Fundamental Organic Chemistry

25 September 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

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

51th 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 Hirosima. In Hirosima 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 acethylformoin 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

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 Takatsuki to Uji. In December, 1970 he was nominated again as the Director, and he aided in the solu-

tion 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 $X\alpha$ (DV- $X\alpha$) 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- $X\alpha$ method.

Dr. Nakamatsu served a Secretary and the member of the Steering Committee of the Society for Discrete Variational $X\alpha$ form 1989. For his scientific achievements and contributions to the Society, he was awarded the Special Prize from the Society for Discrete Variation $X\alpha$ in June, 2004.

Publications International RESEARCH COLLABORATIONS

THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY — Organoelement Chemistry —

Nagahora N, Sasamori T, Takeda N, Tokitoh N: A Kinetically Stabilized Ferrocenyl Diphosphene: Synthesis, Structure, Properties, and Redox Behavior, *Chem. Eur. J.*, 6146-6154 (2004).

Kajiwara T, Takeda N, Sasamori T, Tokitoh N: Unprecedented Insertion Reaction of a Silylene into a B-B Bond and Generation of a Novel Borylsilyl Anion by Boron-Metal Exchange Reaction of the Resultant Diborylsilane, *Chem. Commun.*, 2218-2219 (2004).

Kajiwara T, Takeda N, Sasamori T, Tokitoh N: Insertion of an Overcrowded Silylene into Hydro- and Haloboranes: A Novel Synthesis of Silylborane Derivatives and Their Properties, *Organometallics*, **23**, 4723-4734 (2004).

Mizuhata Y, Takeda N, Tokitoh N: Reduction of Bis(Bromo(Mesityl){2,4,6-Tris[Bis(Trimethy-Isilyl) Methyl]Phenyl}Silyl)Butadiyne with Potassium Graphite: Unexpected Formation of 2-Allenyl-1-Benzosilole, *Phosphorus, Sulfur and Silicon*, **179**, 947-948 (2004).

Tokitoh N, Nagata N, Takeda N: Synthesis and Properties of the First Disulfur and Diselenium Complexes of Platinum, *Phosphorus, Sulfur and Silicon*, **179**, 915-927 (2004).

Takeda N, Hamaki H, Tokitoh N: Synthesis of a Chelate Ring Compound Containing a Lithium Atom by Taking Advantage of a New Unsymmetrical β -Diketiminate Ligand Bearing Bulky Substituents, *Phosphorus, Sulfur and Silicon,* **179**, 727-728 (2004).

Mizuhata Y, Takeda N, Sasamori T, Tokitoh N: Generation of 1,6-Disilahexapentaene in the Reduction of an Overcrowded Bis(bromodiaryl)butadiyne Leading to the Unexpected Formation of 2-Allenyl-1-benzosilole, *Chem. Lett.*, **33**, 420-421 (2004).

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"Structural and Biological Studies on Lectins from the Roots of

Pokeweed (Phytolacca americana)'

Supervisor: Prof OKA, Atsuhiro and Prof HATA, Yasuo

23 March 2004

HORI, Yuichiro

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. Kvoto University

"Synthesis, Antitumor Activity and DNA Interaction of Nitro-5-

deazaflavin Derivatives as New Bioreductive Drug"

Supervisor: Prof SUGIURA, Yukio

23 March 2004

KITANO, Tsuyoshi

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 85Rb"

Supervisor: Prof MATSUKI, Seishi

23 March 2004

MASUNO, Atsunobu

D Sc, Kyoto University

"Control of Physical Properties in Micro-fabricated Perovskite-

type Manganite Thin Films"

Supervisor: Assoc Prof TERASHIMA, Takahito

24 November 2004

MIYAKE, Kousaku

D Sc, Kyoto University

"Magnetism and Magnetoresistance of Magnets with Nano-

contacts Prepared by Nanofabrication Technique"

Supervisor: Prof MIBU, 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, Nobuaki

D Eng, Kyoto University

"Structure Formation and Microscopic Dynamics of Poly(vinyl

alcohol) Gels"

Supervisor: Prof KANAYA, Toshiji

23 March 2004

TAKEBAYASHI, Yoshihiro

D Sc, Kyoto University

"Dipolar Hydration Structure from Ambient to Supercritical

Conditions"

Supervisor: Prof NAKAHARA, Masaru

24 May 2004

TAKEHASHI, 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

TERASAKA, Tadatsugu

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, Yun-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

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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 Eu²⁺-doped Thiogallate Phosphors" Supervisor: Prof YOKO, Toshinobu 24 November 2004

THE 104TH ICR ANNUAL SYMPOSIUM

Seminars Meetings and symposiums

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 Oligosilanes Based on Bicyclic Structure"

HIRATAKE, Jun (Chemistry of Molecular Biocatalysts)
"Design of Enzyme Inhibitors to Probe Enzyme Structure an

"Design of Enzyme Inhibitors to Probe Enzyme Structure and Mechanism"

OKAZAKI, Masaaki (Organotransition Metal Chemistry)
"Stepwise Bromination of Two Acetylene Molecules on a
Tetrairon Core. Formation and Reactivity of Bromoacetylene
- and Dibromoacetylene - Coordinated Clusters"

YOSHIDA, Hiroyuki (Molecular Aggregation Analysis) "Deposition of Acrylonitrile Cluster Ions on Solid Substrates"

NEMOTO, 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

W : Laboratory Whole Presentation

: Laboratory Topic

GE : General Presentation

- The ICR Award for Students -

SHINOHARA, Akihiro (Organoelement Chemistry)

"Synthesis of Kinetically Stabilized Silaaromatic Compounds and Their Properties"

- The ICR Award for Students -

SAITO, Shigeki (Chemistry of Molecular Biocatalysts) "Arabidopsis CYP707As Encode (+)-Abscisic Acid 8'-Hydroxylase, a Key Enzyme in the Oxidative Catabolism of Abscisic Acid"

- Organoelement Chemistry -

- W "Synthesis of Novel Organic Compounds Containing Heavier Elements Ustilizing Kinetic Stabilization and Their Properties"
- ©E MIZUHATA, Yoshiyuki
 "Synthesis of Stable Tin-Carbon Double-Bond Compounds and Stannaaromatics Utilizing Kinetic Stabilization"
- ©E SUGIYAMA, Yusuke
 "Synthesis of a Dibromodigermene Derivative Utilizing
 Kinetic Stabilization and Its Reactions"
- © SHIMIZU, Daisuke
 "Synthesis of Novel Polythioether Ligands Bearing Bulky
 Substituents and Their Complexation with Late Transition

- Structural Organic Chemistry -

- II OGAWA, Kohei; KITAGAWA, Toshikazu; KOMATSU, Koichi
 - "Generation and Properties of a Cyclopentadienyl Cation Annelated with Homoadamantene Frameworks"
- ELEE, Yangsoo; MASAOKA, Naoki; KITAGAWA, Toshikazu; KOMATSU, Koichi
 - "Alkylfullerenyl Cations: Their Generation, Isolation, and Stability"
- - "NMR Observation of 2-Silaimidazolium Cation and Properties of the Related Compounds"
- MAEDA, Shuhei; MURATA, Michihisa; MURATA, Yasujiro; KOMATSU, Koichi
 - "Encapsulation of Molecular Hydrogen into an Open-Cage C_{70} Derivative"

- Synthetic Organic Chemistry -

GE TANIMA, Daisuke

"Temperature Dependent Visual Enantiomeric Recognition by Phenolphthalein Derivatives"

GE MONGUCHI, Daiki

"Asymmetric Cyclization Based on Dynamic Chirality of Englates"

- Chemistry of Polymer Materials -

IT OHKURA, Masahiro

"Material Design Using Fine Particles Coated with High Density Polymer Brushes"

Œ KWAK, Yungwan; GOTO, Atsushi; FUKUDA, Takeshi "Kinetic Studies on Activation Processes in Organotellurium- and Organostibine-Mediated Living Radical Polymerizations"

GE KOH, Kyoungmoo

"Precision Synthesis and Applications of Tadpole-Shaped Polymers with a Fluorine-Carrying Silsesquioxane"

- Chemistry of Polymeric Functionality Materials -

- We "Recent Studies in the area of Chemistry of Polymeric Functionality Materials"
- GE YOSHIOKA, Taiyo; FUJIMURA, Takashi; TSUJI, Masaki; KOHJIYA, Shinzo "Morphological Study on Crystalline Thin Films of PBT"
- MATSUDA, Shota; SENOO, Kazunobu; KOHJIYA, Shinzo
 "Physical Gelation of Syndiotactic Polystyrene in the
 Presence of Poly(ethylene oxide)"

 MATSUDA, Shota; SENOO, Kazunobu; KOHJIYA, Shinzo
 "Physical Gelation of Syndiotactic Polystyrene in the
 Presence of Poly(ethylene oxide)"

 MATSUDA, Shota; SENOO, Kazunobu; KOHJIYA, Shinzo

 "Physical Gelation of Syndiotactic Polystyrene in the
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 MATSUDA, Shota; SENOO, Kazunobu; KOHJIYA, Shinzo

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 MATSUDA

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 "Physical Gelation of Syndiotactic Polystyrene in the Presence oxide oxide

— Inorganic Photonics Materials —

IT KUNIYOSHI, Minoru

"Preparation of Organic-Inoraganic Hybrid Polysiloxane Low-Melting Glasses with High Ultraviolet Transparency"

GE IKAWA, Hiroyuki

"Optical Characterization of the Space Charge Layer in Thin Film TiO₂ Electrodes"

GE MASAI, Hirokazu

"Effect of the Organic Groups on the Formation of Siloxane Network through Gel-Melting Method"

GE HIDAKA, Kenji

"Preparation of Sandwich-type TiO₂/M_mO_n/TiO₂ (M=V and Cr) Multilayer Thin Film Electrodes Via Sputtering Method"

- Magnetic Materials -

W "Spin Induced Transport Phenomena in Nano-scale Ferromagnets"

IT HIMENO, Atsushi

"Ratchet Effect of a Magnetic Domain Wall in Submicron Magnetic Wires with Asymmetric Periodical Notches"

- Biofunctional Design-Chemistry -

II HIRATA, Tsuyoshi

"50 Base Pairs Recognition and Altered DNA Binding Mode by the Longest Artificial 15-Zinc Finger Protein"

GE MASUI, Yumi

"Improvement of Transfection Efficiency by the Addition of pH-sensitive Peptide"

— Chemistry of Molecular Biocatalysts —

II SHIMIZU, Bun-ichi; TAMAI, Michiko; KAI, Kosuke; SAKATA, Kanzo

"Tracer Analysis of the Oxidation Steps in Biosynthesis of Coumarins in Sweet Potato Using ¹⁸O₂"

IT FUJITA, Satomi; OHNISHI, Toshiyuki; WATANABE, Bunta; MIZUTANI, Masaharu; SAKATA, Kanzo "Biochemical Analysis of Plant Cytochrome P450 Monooxygenases in Brassinosteroid Biosynthesis"

— Molecular Biology —

IT OKA, Atsuhiro; AOYAMA, Takashi; YASUDA, Keiko; TANIGUCHI, Masatoshi

"Function and Target Gene Analyses of the *Arabidopsis* Response Regulator ARR1 Capable of Transactivation"

GE TSUGE, Tomohiko; OKA, Atsuhiro

"CSN: The Key Complex Linking Environmental Signals to Morphogenesis in Plants"

GE IMAI, Kumiko

"Function Analysis of AtCYCA2;3 in Regulation of Endoreduplication"

- Molecular Clinical Chemistry -

Œ TAKAGI, Junpei; TAKEHASHI, Masanori; TANAKA, Seigo

"Mitochondrial Impairment Induced by Poly(ADP-ribose) polymerase-1 Activation after Cerebral Ischemia"

GE TAKEHASHI, Masanori; TANAKA, Seigo

"Expression and Complex-formation of Brain-specific Protein Septin 3"

- Molecular Materials Chemistry -

T YAMADA, Tomonori; TSUKAMOTO, Naoki; KUSAKA, Yasunari; KAJI, Hironori; HORII, Fumitaka

"Precise Structure Analysis of Organic EL Materials by Solid-State NMR and Quantum Chemical Calculations"

II SUZUKI, Furitsu; TSUJITANI, Kouji; HIRAI, Asako; HORII, Fumitaka

"Structure and Structural Change of Sub-elementary Fibrils of Bacterial Cellulose in an Initial Period of Layered System Organization"

- Hydrospheric Environment Analytical Chemistry -

IT NORISUE, Kazuhiro

"Distribution of Trace Metals in the Sulu Sea and Its Adjacent Basins"

GE SASAKI, Yoshihiro

"Minimal Mode Simulated in Kicked Oscillators"

- Solution and Interface Chemistry -

II OKAMURA, Emiko; WAKAI, Chihiro; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru "Molecular Dynamics in Lipid Membranes and Drug Delivery by NMR"

© NAGAI, Yasuharu; MOROOKA, Saiko; MATUBAYASI, Nobuyuki; NAKAHARA, Masaru "Noncatalytic Reactions of Aldehyde and Ether in Supercritical Water"

— Molecular Microbial Science —

IT KUROKAWA, Suguru

"Physiological Function of Selenocysteine Lyase"

GE KAWAMOTO, Jun

"Proteome Analysis of a Psychrotrophic Bacterium, Shewanella sp. Ac10, to Elucidate Its Cold-adaptation Mechanism"

- Polymer Materials Science -

- "Accurate Analysis for Higher Order Polymer Structure"
- Œ KAWAI, Takahiko; STROBL, Gert; KANAYA, Toshiji "Crystallization of a Poly(ethylene-co-octene): A Precursor Phase and two Competing Mechanisms"

- Molecular Rheology -

- "Perspective of Molecular Rheology"
- GE KIKUCHI, Toshimitsu

"Electric Birefringence of Amorphous Polymers"

- Molecular Aggregation Analysis -

YAMAGUCHI, Takayuki "Molecular Photoelectron Spectroscopy of BMDCM"

GE ASAMI, Koji

"Dielectric Relaxation in Microemulsions Near Temperaturedependent Phase Inversion"

- Supramolecular Biology -

TAKAHARA, Keigo; TAKEUCHI, Ken-ichi; UMEDA Masato "The Role of Fatty Acid Desaturase in Energy Metabolism of Organisms" TANIUCHI, Kentaro; INADOME, Hironori; KATO, Utako; TAKEUCHI, Ken-ichi; UMEDA, Masato "Regulation of Cell Morphology and Cell Size in Multicellular Organisms"

— Particle Beam Science —

GE YAMAZAKI, Atsushi

"Generation of a Monoenergetic Electron Beam Using a Single Laser Pulse"

GE FUJIMOTO, Shinji

"Non-destructive Beam Monitor Development for a Small Ion Storage Ring S-LSR"

GE TAKEUCHI, Takeshi

"Magnetic Field Measurement of Quadrupole Magnets and Accelerator Alignment for S-LSR"

GE TONGU, Hiromu

"Improvement of Beam Lifetime in the Electron Storage Ring, KSR"

Œ TANABE, Mikio; SHIRAI, Toshiyuki; IKEGAMI, Masahiro; TONGU, Hiromu; NODA, Akira "Design of the Deflection Elements for Dispersion Control"

— Laser Matter Interaction Science —

GE SHIMIZU, Seiji

"Desorption/ionization Induced by an Intense Short Pulse Laser"

- Electron Microscopy and Crystal Chemistry -

- W "Research Topics in Our Laboratory"
- GE MINARI, Takeo

"Organic Field-effect Transistor Based on Single-grain Pentacene"

- Structural Molecular Biology -

IT FUJII, Tomomi; HATA, Yasuo

"Structure of the Complex between Carboxypeptidase Y and its Protein Proteinase Inhibitor IC"

- Organic Main Group Chemistry -

GE MATSUNAGA, Tadafumi

"Cross-coupling Reaction of Aryl- and Alkenyl-trifluorosilanes with 1-aryltriazenes Using a Palladium Catalyst"

GE SASE, Shohei

"Synthesis of Disilatriptycene Oligomers"

— Advanced Solid State Chemistry —

- Transition Metal Oxides Functions and Synthesis -"
- GE 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-x}CuO₂Cl₂"

- Organotransition Metal Chemistry -

"International Research Center for Elements Science, Organotransition Metal Chemistry: Research Topics in 2004"

E KATAYAMA, Hiroyuki

"(Z)-Selective Cross-dimerization of Arylacetylenes with Silylacetylenes Catalyzed by Vinylideneruthenium Complexes"

- Bioknowledge Systems -

William Bioknowledge Database KEGG and Its Application to Bioinformatics"

GE KOTERA, Masaaki

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

— Biological Information Network —

[W] "Computational Analysis of Structures of Biological Information Networks and Chemical Compounds"

- Bioinformatics Training Unit -

II KATOH, Kazutaka

"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 BANKAITIS, Vytas 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. Universite Bordeaux I, France

"Modeling Time-Resolved Spectroscopies HDO in D₂O or A Very Simple Model of Intermolecular Energy Relaxation in Order to Study Energy Flows in Liquids"

10 June 2004

Prof CHHABRA, 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 DIBO, 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

"Magneto-optical 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 FRIEDLEIN, 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-Iion 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 Nucling"

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 GRIESER, 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

"Studing Ferromagnetism with Combined Magnetic Force Microscopy and Magnetiresistance 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 Swichable Properties"

17 November 2004

Dr HANAGURI, Tetsuro

Magnetic Materials Laboratory, RIKEN, Wako, Japan

"STM/STS Studies on a Lightly-doped Cuprate Ca_{2-x}Na_xCuO₂Cl₂"

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 Em HORIE, Kazuyuki

The University of Tokyo, Tokyo, Japan

"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-rage Free-Electron Laser and its Application"

5 January 2004

Prof KAGAN, Henri Boris

Institut de Chimie Molculaire et des Materiaux, Universite 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

"Magneto-science and Magnetochemistry"

12 March 2004

Dr KRAKOVSKY, Ivan

Charles University, Czech Republic

"Structure and Properties of Hydrophilic Epoxy Networks" 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, Kitae

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. F

"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-(carbomethoxy)triazolines Involving Intramolecular 1,3-Dipolar Cycloreversion"

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

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"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 NICLES, 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- $T_{\rm C}$ 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 Perfluorinated 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 STANGER, Amnon

Technion (Israel Institute of Technology)

"Another Story of Aromaticity that is Told by Strained Aromatic Compounds"

12 February 2004

Prof STREUBEL, 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, Warszawa, 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

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, Katsunori

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 h5-Coordinating Ligands. Regioselective Monoalkylation and Monoarylation in Cobaltabisdicarbollide [3,3'-Co(1,2-C₂B₉H₁₁)₂]- Clusters" 6 December 2004

Dr TONGE, Matthew P.

UNESCO Center of Macromolecules and Materials, Stellenbosh 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 WEST, 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-Demensional 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 Prof YOUNG, Petey Southern Oregon University, USA "Writing for Publication in English" 16 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 TAMAO, Kohei 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 Nanoscaled Molecular Clusters: From Dipolar Molecules to Aromatic Molecules"

Prof BERTRAND, Guy

University of California, Riverside, USA

"Stable Singlet Diradicals and Tetraradicals 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 Hexaboride KB6"

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 κ -(ET)₂Cu₂(CN)₃"

Prof GULDI, Dirk M.

University of Notre Dame, USA

"Novel Multifunctional Nanoarchitectures 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 TOKITOH, 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 Porphyrinoids; *Meso-meso* Coupled Porphyrin Arrays and Expanded Porphyrins"

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, Kvoto 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 Mibu

"Magnetism and Magnetoresistance Effect of NiFe Wires or Dots with Nanocontacts"

Takuva Okuno and Ko Mibu

"Temperature Dependence of Switching Field of Turned-up Magnetization in CoNbZr Circular Dots"

Takuo Ohkochi, Ko Mibu, Nobuyoshi Hosoito, and Hiroo Hashizume

"Induced Spin Polarization in Non-magnetic Layers of Magnetic/ Non-magnetic Metallic Multilayers"

Norihiro Jiko and Ko Mibu

"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 BiNiO3"

Seiji Niitaka, Masaki Azuma, Mikio Takano, Eiji Nishibori, Masaki Takata, and Makoto Sakata

"High-pressure Synthesis and Physical Properties of Bi-contained Transition Metal Oxides BiCrO₃ and BiCoO₃"

Dan Wang, Ranbo Yu, Masaki Azuma, Takahito Terashima, and Mikio Takano

"Solvo-Thermal Synthesis of Novel Low-Dimensional Zirconium Phosphates"

Daisuke Kan, Takahito Terashima, Mikio Takano, and Akio Yamanaka

"Preparation and Optical Properties of Single-Crystalline CaCuO₂ Thin Film with Infinite Layer Structure"

Atsushi Ishizumi, Hiroki Matsubara, and Yoshihiko Kanemitsu "Optical Properties of Semiconductor Nanocrystals Doped with Luminescence Centers"

Hideyuki Inouye, 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, Yomei Tokuda, and Toshinobu Yoko

"Formation of Organic-inorganic Hybrid Low-melting Glasses Via Acid-base Reaction of Phosphoric Acid and Chlorosilane"

Masanori Saito, Hiroshi Kakiuchida, Yomei Tokuda, Masahide Takahashi, and Toshinobu Yoko

"Laser Fabrication of Organic-inorganic Hybrid Low-melting Glass Prepared through Non-aqueous Acid-base Reaction"

Yomei Tokuda, Masahide Takahashi, and Toshinobu Yoko "Inhomogeneous Distribution of Local Structures around Na Ion in Silicate Glasses by ²³Na MQMAS NMR Spectroscopy"

Masahide Takahashi, Yomei Tokuda, and Toshinobu Yoko "Photochemical Reactions Responsible for Photorefractive Index Change in Germanosilicate Glasses"

Hirokazu Masai, Masahide Takahashi, Yomei Tokuda, and Toshinobu Yoko

"Effect of the Organic Groups on the Formation of Siloxane Network"

Dorjpalam Enkhtuvshin, Masahide Takahashi, and Toshinobu

"Effects of the Accumulated VO₂-rich Regions on the Photoelectrochemical Performance of the Sol-gel Derived $Ti_{0.95}V_{0.05}O_2$ Thin Film Electrodes"

Youichiro 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 Neilands

"Changes in Crystal Structure and Solid State Properties of a Zwitterionic Compound by Its Aza Substitution"

Kazukuni Nishimura, Gunzi Saito, Chin Hong Chong, Masaru Makihara, Salavat Khasanov, Hideki Yamochi, Akihiro Otsuka, Kenji Kamada, Koji Ohta, and Jun Kawamata

"The Estimation of Intramolecular Ionicity, Dipole Moments and (Hyper)polarizabilities in the D $^{\delta+}$ - π -A $^{\delta-}$ Zwitterions Prepared from Indoline and TCNQ Derivatives"

Hideki Yamochi, Akira Ota, and Gunzi Saito "Status of (EDO-TTF)₂PF₆ at Present"

Masafumi 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, Kazuya Miyagawa, and Kazushi Kanoda

"Role of Anisotropy in the κ -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"

Tsuyoshi Haneda, Hideki Yamochi, Gunzi Saito, Adam Tracz, Jacek Ulanski, Olga Drozdova, and Kyuya Yakushi

"Humidity Sensitive Conductivity of (BEDO-TTF)₂Br(H₂O)₃ as a Bulk Property"

Junichi Fujii, Yukihiro Yoshida, Koji Muroi, Akihiro Otsuka, and Gunzi Saito

"1-Ethyl-3-methylimidazolium Based Ionic Liquids Containing Cyano Groups: Synthesis, Physical Property and Crystal Structure"

Yoshikazu Umemoto, Yasushi Morita, Eigo Miyazaki, Suguru Maki, and Kazuhiro Nakasuji

"Syntheses and Physical Properties of an Ethylenedithio-TTF Derivative with Butyluracil and Its CT Complexes"

Takeshi Ishiyama, Shogo Yamamoto, and Fumiyuki Ozawa "Synthesis and Reactions of Hydridoplatinum(II) Complexes Bearing Diphosphinidenecyclobutene (DPCB) Ligands"

Takashi Sagawa and Fumiyuki Ozawa

"Alkyne-Insertion into Group 14 Element Platinum Bonds"

Hiroyuki Katayama, Yosuke Fukuse, Masato Nagao, and Fumiyuki Ozawa

"Highly Selective Ring-Opening Cross-Metathesis Reactions Using Fischer-type Carbene Ruthenium Catalysts"

Masaki Shimizu, Xinyu Liu, and Tamejiro Hiyama

"A Facile Stereocontrolled Approach to CF₃-Substituted Triarylethenes"

Masaki Shimizu, Masanori Nata, Kotaro Watanabe, and Tamejiro Hiyama

"Novel Liquid Crystalline Compounds Based on 1-Aryl-2,3,5,6,7,8-hexasilabicyclo[2.2.2]octanes"

Yoshiaki Nakao, Jun Satoh, Eiji Shirakawa, and Tamejiro Hiyama

"Palladium-Catalyzed Decarbonylative Carbostannylation of Propargyl Esters"

Yoshiaki Nakao, Shinjiro Ishihara, Yasuhiro Hirata, Shinichi Oda, Yuki Honda, Eiji Shirakawa, and Tamejiro Hiyama

"Palladium Iminophosphine-Catalyzed Stannylative Cyclization of Conjugated Enynes and Diyne"

Masaki Shimizu, Takuya Kurahashi, Hirotaka Kitagawa, Katsuhiro Shimono, and Tamejiro Hiyama

"gem-Silylborylation Approach to Tri- and Tetrametalmethanes: the First Synthesis of Boryl(germyl)(silyl)(stannyl)methanes"

Hideki Amii, 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 Sugiura

"Intracellular Delivery of RNase S Complex Bearing Arginine-rich Peptides"

Wataru Nomura and Yukio Sugiura

"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 Terthiophene- Fullerene Dyads"

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

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

Rika Nogita, Tohru Nishinaga, Daisuke Yamazaki, and Koichi Komatsu

"Synthesis and Properties of Bis(bicyclo[2.2.2]octeno)TTF"

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

Shuichi Suzuki, Yasushi Morita, Kozo Fukui, Hiroshi Kitagawa, Hideo Kishida, Hiroshi Okamoto, Akira Naito, Shigeaki Nakazawa, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, and Kazuhiro Nakasuji

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

Noriyoshi Nagahora, Takahiro Sasamori, Nobuhiro Takeda, and Norihiro Tokitoh

"Synthesis, Structure, and Properties of a Novel Ferrocenylsubstituted Diphosphene 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 Norihiro Tokitoh "Synthesis and Properties of the First Monomeric, Donor-free Lithium β- Diketiminates Stabilized by Bulky Substituents"

Yutaka Ishida and Akira Sekiguchi

"Synthesis, Structure, and Reaction of First Germanium Bishomoaromatic Cation"

Atsushi Wakamiya, Toshihisa Ide, and Shigehiro Yamaguchi "Synthesis and Properties of Trianthrylborazines"

Caihong Xu, Atsushi Wakamiya, and Shigehiro Yamaguchi "Benzo[b]silole as a New Building Unit for Fluorescent π -Conjugated Systems"

Shigehiro Yamaguchi, Masataka Miyasato, and Kohei Tamao "Reductive Bergman-Type Cyclization of Cyclic 1,2-Bis(silylethynyl)benzenes" Tomoyuki Saeki, Eun-Cheol Son, Tadafumi Matsunaga, and Kohei Tamao

"Palladium Catalyzed, Lewis Acid Induced Cross-Coupling Reaction of 1- Aryltriazenes with Areneboronic Acids and Aryltrifluorosilanes"

Hayato Tsuji, Deborah L. Casher, Martins Katkevics, Mari Kubota, Tsunetoshi Kobayashi, Akio Toshimitsu, Josef Michl, and Kohei Tamao

"Relationship between Structure and Photophysical Properties of Peralkylated Disilanes"

Hayato Tsuji, Motoki Toganoh, Takeshi Kataoka, Yuki 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 TOKITOH, Norihiro; TAKEDA, Nobuhiro; TAMAO, Kohei; TSUJI, 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, Yushu

Nagoya University

"Microdomain Structures of Block Copolymers with Wide Composition Distribution"

Prof TSUJII, Yoshinobu

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

Kvoto 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, Mitsuhiro

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 Ionisable 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

Nambu T, Yamauchi Y, Kushiro T, Sakurai S

Kyoto Institute of Technology, JPN

"Micro-convection, Dissipative Structure and Pattern Formation in Polymer Blend Solutions under Temperature Gradients"

Hayashi K, Kizaki S, Sakurai S, Ejima Y*1, Shimizu T*1, Hara S*2, Yamamoto K*2, Okamoto S*2

Kyoto Institute of Technology, JPN, KANEKA Corporation, JPN*1, Nagoya Institute of Technology, JPN*2

"Simultaneous SAXS/WAXS/Hv-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*1, Kyoto University, JPN*2 "Thermal Expansion Behavior of Thin Polymer Films"

Takeshita H, Takenaka K, Shiomi T

Nagaoka 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.*3, Levett S. J.*3

Kyoto University, JPN, Chiba Institute of Technology, JPN*1, JAERI, JPN*2, Rutherford Appleton Laboratory, UK*3

"Inelastic Neutron Scattering from Polystyrene Thin Films"

Matsuba G, Ogino Y, Sakamoto S, Kanaya T, Nishida K Kyoto University, JPN

"Shish-kebab Structure in the Drawing Polyethylene Blends with Ultra-high Molecular Weight Component"

Yamauchi Y, Kizaki S, Yokotani K, Sakurai 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, Matsuba G, Kanaya T

Kyoto University, JPN

"Crystallization and Mesomorphic Phase Formation of Isotactic Polypropylene"

Ogino Y, Matsuba G, Sharma L, Nishida K, Kanaya T

Kyoto University, JPN

"Crystallization of Isotactic Polypropylene under Shear Flow"

Akemura M, Munakata S, Sakurai S

Kyoto Institute of Technology, JPN

"Effects of the Pressure on Regularity of Cylindrical Microdomains in Block Copolymers"

Senoo K, Atsumi K, Kohjiya S, Ikeda Y*

Kyoto University, JPN, Kyoto Institute of Technology, JPN*
"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, Matsuba 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, Sakurai S

Kyoto Institute of Techonology, 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*1

Nara National College of Technology, JPN, Osaka Prefecture University, JPN*1, Osaka Institute of Technology, JPN*2 "Molecular Design of Thermoresponsive Polypeptides"

Hirano Y, Okada M, Iuchi T, Kakinoki S*1, Oka M*1
Osaka Institute of Technology, JPN, Osaka Prefecture University,

"Synthesis and Conformational Analysis of Poly(dipeptide)s"

Kakinoki S, Teraoka M, Onoda Y, Oka M, Hirano Y*1

Osaka Prefecture University, JPN, Osaka Institute of Technology, IPN*1

"Synthesis and Conformational Analysis of Poly(tripeptide)s"

Kakinoki S, Yuge M, Arimoto M, Teraoka M, Oka M, Hirano Y*1 Osaka Prefecture University, JPN, Osaka Institute of Technology, JPN*1

"Synthesis and Conformational Analysis of Poly(tetrapeptide)s"

Kawaguchi T, Nozaki Y, Kaneko F

Osaka University, JPN

"Structure Research of Dialkyl-1,18-octadecanedioate"

Shirouchi K, Munakata S, Sakurai S, Kurimura H*, Suzuki S* Kyoto Institute of Technology, JPN, Denki Kagaku Kogyo, K.K.* "Features of Microphase-separated Structures in S₁BS₂ Triblock Copolymers with Different Lengths of End-block Chains"

Funai E, Sakurai S, Okamoto S *1 , Yamato M *2 , Kimura T *2 Kyoto Institute of Technology, JPN, Nagoya Institute of Technol

ogy, JPN*1, 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, Tsujii Y, Fukuda T, Torikai N*1, Takeda M,*2 Kyoto University, JPN, High Energy Accelerator Research Organization, JPN*1, JAERI, JPN*2

"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, Ohno K, Tsujii Y, Fukuda T, Yamahiro M*, Ootake N*, Watanabe K*
Kyoto University, JPN, Chisso Petrochemical Co., JPN*
"Synthesis of Tadpole-Shaped Polymers with Polyhedral Oligomeric Silsesquoxane"

Yoshikawa C, Goto A, Tsujii Y, Fukuda T, Yamamoto K^* , Kishida A^*

Kyoto University, JPN, National Cardiovascular Center Research Institute, ${\rm JPN}^*$

"Precise Surface Design with High-Density Polymer Brushes: Application to a Polymeric Film"

Ogawa H*1.2, Norisuye T*2, Tran-Cong-Miyata Q*2 Kyoto University, JPN*1, Kyoto Institute of Technology, JPN*2 "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)



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