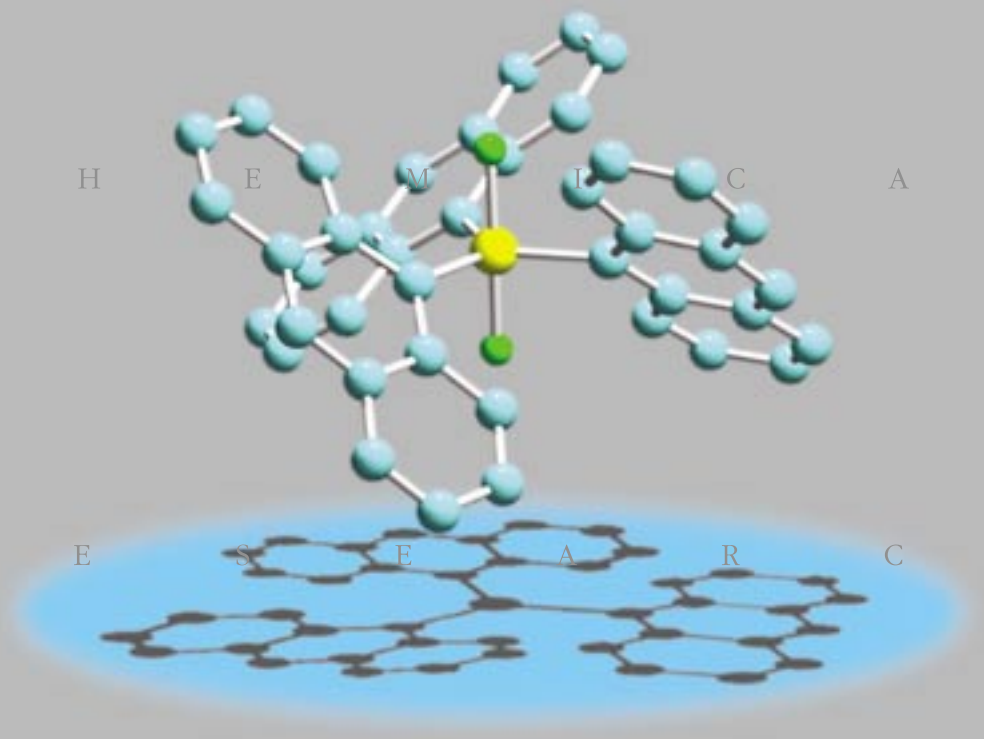
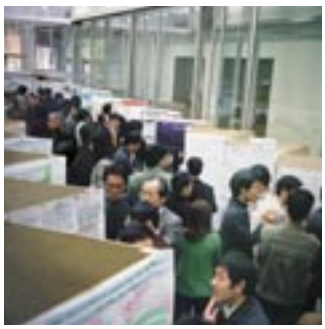
INSTITUTE FOR CHEMICAL RESEARCH



KYOTO UNIVERSITY

Institute for Chemical Research
Kyoto University
2003



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Preface

Director
TAKANO, Mikio

The Institute for Chemical Research (ICR) of Kyoto University celebrated its 77th anniversary in 2003. The ICR had its origin in a laboratory created in 1915 in the College of Science to study and manufacture salvarsan and was formally founded in 1926 as the first university-affiliated research institute in Japan. For 77 years, we have made many significant contributions to the development of science and technology through a wide range of research with our own original ideas based on the noble doctrine, "Conducting Fundamental Studies and Exploring Their Application to Special Fields of Chemistry".

Some of the latest evolutionary changes in the ICR will be enumerated below. In 2001 the "Bioinformatics Center" was established, and in April of this year the "International Research Center for Elements Science" was just established. The ICR now includes nine divisions and three affiliated research centers, which consists of a total of 31 laboratories and five guest-laboratories with almost one-hundred researchers included. The activities of these laboratories encompass organic chemistry, inorganic chemistry, biochemistry, materials chemistry, and physical chemistry. Currently, each laboratory is affiliated with one of the Graduate Schools: Science, Engineering, Agriculture, Pharmaceutical Sciences, Medicine, or Informatics.

Our Institute continues a long and proud tradition of hosting many foreign research associates and students and collaborating with overseas researchers in various fields. We encourage students and young researchers by offering the Director Prize for their excellent achievements. And we have strived to improve the public's understanding of chemistry by holding open seminars for the average citizen and high-school students.

The organization of national universities will be significantly changed by transformation into cooperate bodies in April of next year (2004). To meet this inevitable turning point and the changes that lie ahead, we should emphasize more strongly "science for society" in our guiding principle than before: In this aspect such activities as mentioned in the upper paragraph will be of more importance. This does not mean to forget about "science for science", however. To realize our future we believe that it will be important to encourage young researchers to incubate their interdisciplinary and creative ideas in the ICR, a great melting pot, while combining the motivating and inspiring concepts of "science for society" and "science for science".

June, 2003

History

1926.10 The organization of the Institute for Chemical Research (ICR) was published.
It was composed of a director, professors, instructors (full-time), and the secretariat (full-time).
The object was conducting fundamental studies in special fields of chemistry and exploring their application.

1929 The main building of ICR was constructed in Takatsuki, near Osaka.

1962 Association with graduate schools for the education of students was institutionalized.

1964 The Division System was established (19 divisions and 1 satellite facility).
Nuclear Science Research Facility was located at Awataguchi, Sakyo-ku, Kyoto.

1968 Laboratory of High-pressure Electron Microscopy was located at Gokasho, Uji (Uji Campus).
ICR was moved to the Uji Campus.

1971 Low-Temperature Laboratory was established.

1975 Biotechnology Laboratory was established.
Central Computer Facility was located.

1981 Research Facility of Nucleic Acids was established.

1988 Nuclear Science Research Facility was moved to the Uji Campus.

1989 High-resolution electron spectromicroscope was located.

1992 Supercomputer Laboratory was established.
ICR was reorganized into 9 research divisions and 2 satelite facilities.

1999 Joint Research Laboratory was established.

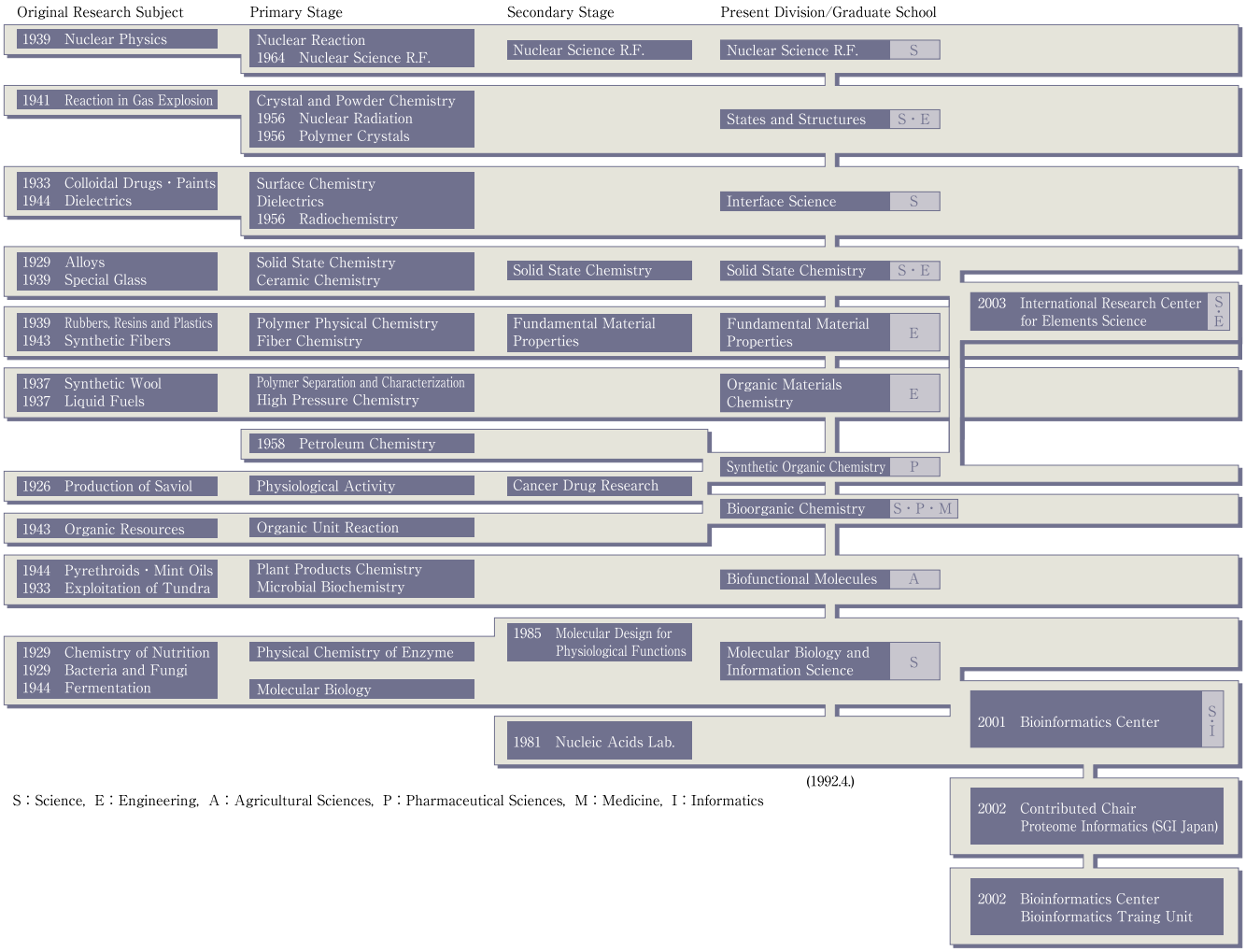
2000 ICR became the epicenter of "Kyoto University COE:Elements Science".
Administration Department was integrated into that of the Uji Campus.

2001 Bioinformatics Center was established.
ICR started a research program "Collaboratory on Electron Correlations - Towards a New Research Network between Physics and Chemistry".

2002 Proteome Informatics Laboratory was donated by SGI Japan.
Bioinformatics Center, Bioinformatics Training Unit was established.
ICR started a COE program for the 21st Century "Kyoto University Alliance for Chemistry".
ICR jointly started a Nanotechnology Support Project of MEXT, Japan, "Precise Analysis Support of Nanosize Materials".

2003 International Research Center for Elements Science was established.
ICR jointly started a new national project : National Research Grid Initiative (NAREGI).
ICR became the epicenter of a COE program for the 21st Century "Center of Research and Knowledge Information Infrastructure for Genome Science".

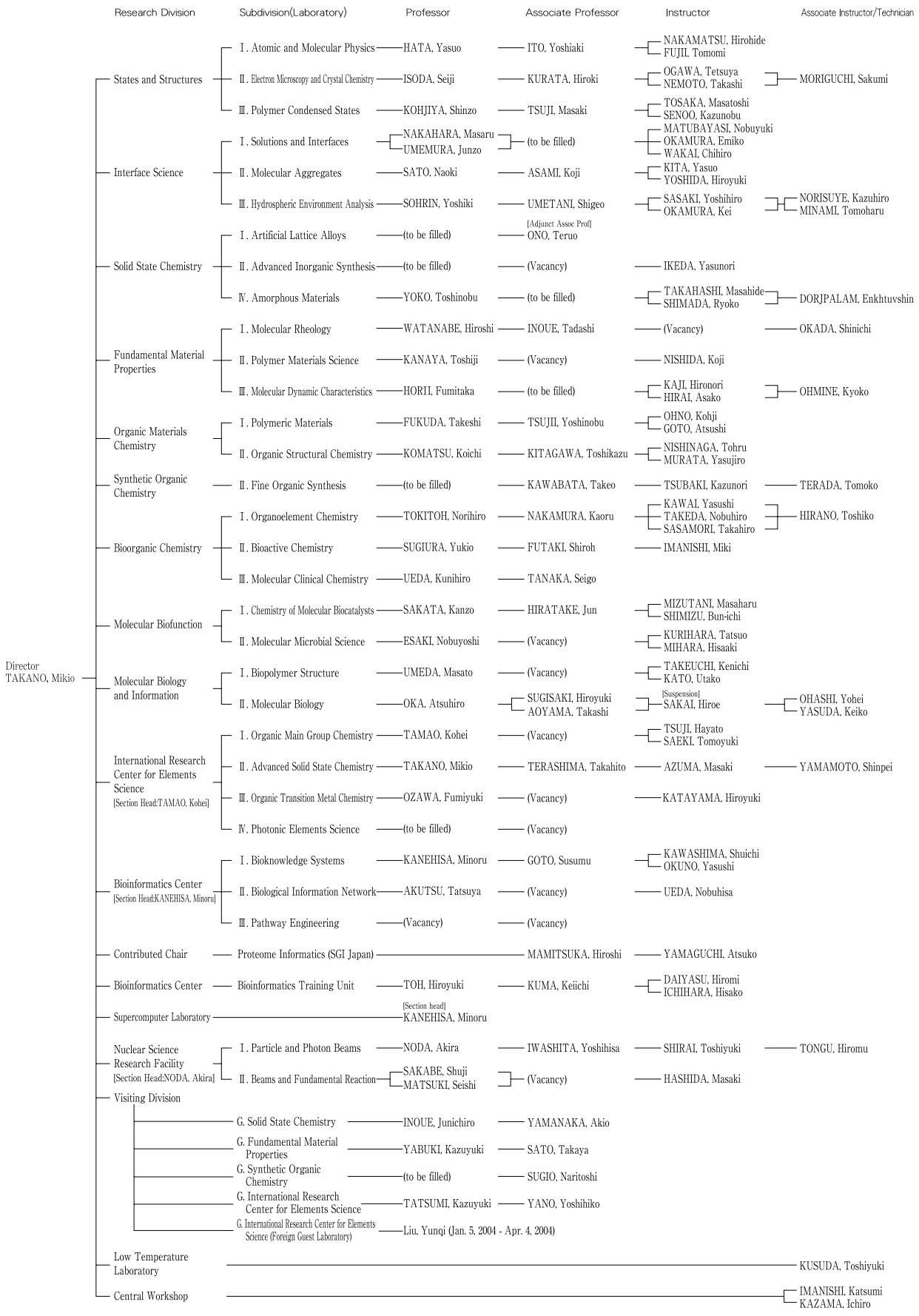
Divisions and Their Historical Backgrounds



S : Science, E : Engineering, A : Agricultural Sciences, P : Pharmaceutical Sciences, M : Medicine, I : Informatics

Organization

(As of September 1, 2003)



(G : Laboratory for Visiting Professor)

STATES AND STRUCTURES I S

Atomic and Molecular Physics

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Detailed information on the structure of the substance can be obtained using X-ray strongly interacting with electrons distributed around the atomic nucleus. This laboratory aims at elucidating the relationships between the structure and the function or properties of functional substances by investigating the electron-density distribution or the electronic states of their atoms and molecules in detail using X-rays from an ordinary generator and synchrotron radiation. The main research subjects are as follows:

(1) X-ray crystallographic structure determination of functional substances and structure-based analysis of their functions. The X-ray crystallographic structure analysis is best for precise and high-resolution structure determination of functional macromolecules. The structure determination of proteins and their complexes, and the structure-based analysis of expression mechanisms of their functions and properties are performed using the X-ray diffraction method.

(2) Investigation of the electronic states of atoms and molecules of materials. In order to obtain fundamental information on the structure and the property of materials, the experimental and theoretical investigation of the natural line width in K and L emission lines by high-resolution X-ray spectroscopy, the theoretical analysis of the electronic states from the X-ray absorption and emission spectra, and the development of the detector for soft X-rays are underway.

Figure legend: Electron density map of a protein molecule

STATES AND STRUCTURES II S

Electron Microscopy and Crystal Chemistry

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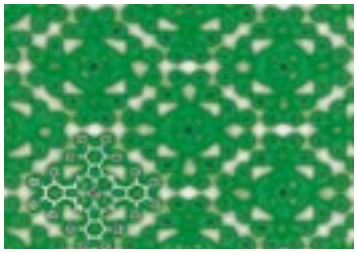
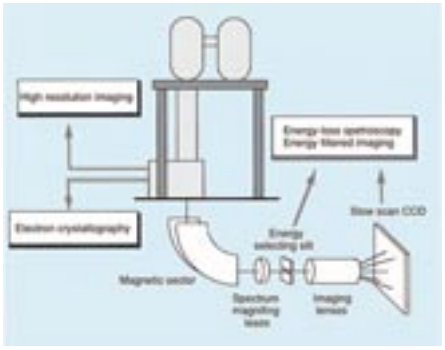
Due to the strong interaction between fast incident electrons and materials, electron microscopic methods are powerful tools to extract information on structural and electronic states of ultra-fine specimens. So as to realize atomic resolution, a 1000 kV electron spectro-microscope has been developed. This electron microscope can resolve atoms or molecules in specimens by using elastically scattered electrons and crystal structures in thin films can be analyzed directly by electron crystallography method as well. In addition to these, inelastically scattered electrons are utilized to investigate the collective motions of electrons in specimens, quantitative elemental distributions, chemical states of bonding, interactions between neighboring atoms and so on. In cooperation with these methods, scanning probe microscopes are also employed to study low dimensional crystallization processes, surface chemical reactions, functionalities of fine particles and thin films.





STATES AND STRUCTURES III E

Polymer Condensed States

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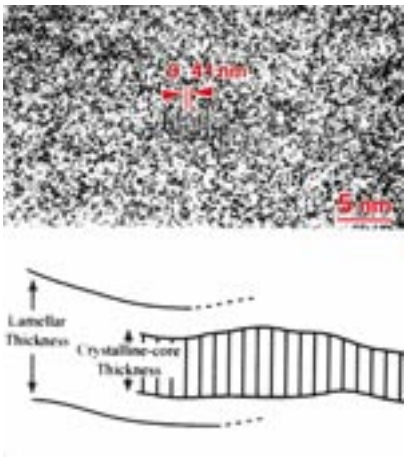
Instructor TOSAKA, Masatoshi (D Eng)
SENOO, Kazunobu (D Eng)

The research at this subdivision is devoted to correlation studies on the structure and properties of polymer condensed states by analyzing chemical and higher-order structures, as well as by measurements of various physical properties. Physical properties of a polymer are determined not only by the chemical structure but also by molecular arrangement in the condensed state including the solid and the liquid. To produce a better polymer material, the knowledge of the structure and its formation mechanism is important. In order to clarify the structures, their formation mechanism and structural changes in molecular dimension, the following studies are currently performed: high-resolution electron microscopy of polymer crystals; in situ light or X-ray scattering/diffraction studies on formation and deformation process of a polymer; structural characterization of polymer gels and elastomeric materials followed by theorization of their mechanical behavior. By exploiting outcomes from these studies, developments of new functional polymer composites and their characterization are also performed.



High-resolution electron micrograph of a poly (3-oxotrimethylene) edge-on lamella crystallized epitaxially from solution on the (001) surface of KI, and the schematic illustration. The crystalline-core thickness of a lamella was revealed to be about one-half of the corresponding lamellar thickness.

INTERFACE SCIENCE I S

Solutions and Interfaces

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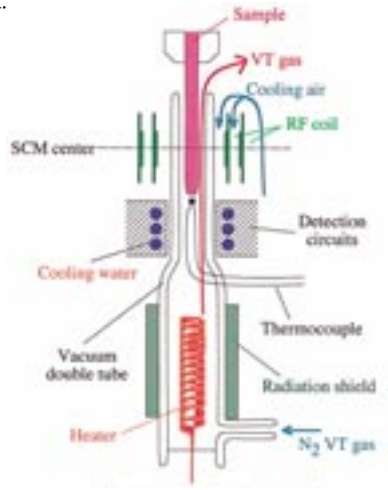
WAKAI, Chihiro (D Sc)

Structure and reactions of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are studied by means of NMR, Raman, and computer simulation under extreme conditions including supercritical and supercooled. A systematic exploration of a wide range of thermodynamic conditions is performed for supercritical fluids to elucidate and control the solute-solvent interaction. Especially, the density of the solvent is varied from the gas-like to liquid-like regimes and a drastic change in the solvation properties is achieved. The dynamics of supercritical fluids, especially of aqueous solutions, is also probed and the effect of the high kinetic energy resulting from the high temperatures involved at supercritical states is characterized. Organic chemical reactions of water and aqueous solutions at super- and subcritical conditions are investigated from the physico-chemical and environmental-science points of view. From the physico-chemical viewpoint, the role of water in organic chemical reactions is specified at the fundamental and molecular level by developing the in-situ NMR spectroscopy. From the environmental-science viewpoint, non-catalytic reactions are pursued in high-temperature water by exploiting the water molecule itself as both the medium and reactant. Especially, the role of high-temperature water as an effective acid or base is revealed and quantified. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Crystallization of protein monolayers, advanced dispersion systems at liquid-liquid interfaces, and biomembranes are also investigated.



High-temperature probe used for in-situ observation of chemical reactions in supercritical water

INTERFACE SCIENCE II S

Molecular Aggregates

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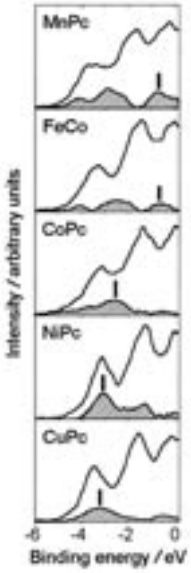
Studies to elucidate correlation between structures and properties of molecular aggregates are carried out in two aspects: solid-state chemistry of organic thin films based on analyses of their electronic and geometrical structures and physicochemistry of polymers, membranes and biomaterials by means of electrical measurements.

The former research aims in principle at creating novel molecular systems with notable electronic functions. Both occupied and unoccupied electronic structures in organic semiconductors are directly observed by photoemission and inverse photoemission spectroscopies, respectively. Correlations of such electronic structures in the films and/or at their interface with molecular orientations in them are of our most interest. With bearing in mind such analytical results, synthetic investigations are also made to build up novel molecular systems by assembling molecules newly selected or designed, e.g., highly amphoteric and polar molecules. Further, organic solid-state reactions attract our attention as promising phenomena inducing dynamic electronic properties, so reaction mechanisms are studied for several systems, e.g., a methylcation transfer system.

The latter research aims to analyze heterogeneous structures particularly in biological membranes and cells, in relation to their functions. Lipid-bilayer and biological membranes with ion-channels are examined in aqueous solution using several electrical methods. Biological cells under specific conditions such as high pressures are also observed in situ with making full use of these methods, e.g., scanning dielectric microscopy. Further, nonlinearity in dielectric properties of condensed molecules is studied in relation to molecular motions.



Inverse photoemission spectra of MPc (M = Mn, Fe, Co, Ni and Cu; Pc = phthalocyanine) thin films. The difference spectra (hatched area) between them and the reference ZnPc one clearly show the density of unoccupied states derived from the central metals; solid bars indicate a systematic energy shift of a particular d-level.

INTERFACE SCIENCE III S

Hydrospheric Environment Analysis

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Technician MINAMI, Tomoharu

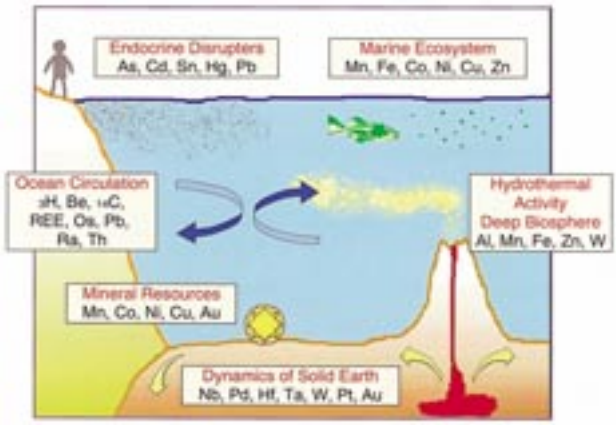
Research activities are concerned with geochemistry, oceanography, limnology, and analytical chemistry, which are important basic sciences in order to realize the sustainable society. Major research subjects are as follows:

(i) Biogeochemistry of trace elements in the hydrosphere. Novel analytical methods are developed for multi-elemental determination, isotope ratio determination, speciation, and in situ measurements. Distribution of trace elements and its effects on ecosystem are investigated. The study also covers hydrothermal activity and deep biosphere. Major parts of these studies are based on field works.

(ii) Iron uptake mechanism of phytoplankton. The ultimate aim of this study is to control photosynthesis of phytoplankton and sequester atmospheric CO_2 in the ocean. As a basic science for this aim, iron uptake mechanism of phytoplankton is investigated. We are pursuing iron transport molecules (siderophores) produced by phytoplankton.

(iii) Ion recognition. Ligands that have novel functions in ion recognition are designed, synthesized, and characterized. The ion recognition systems are applied to the development of separation technology and sensors.

(iv) Simulation of chemical reactions. Instructor Sasaki is studying non-linear chemical reaction in order to understand synchronization and excitation.



SOLID STATE CHEMISTRY I S

Artificial Lattice Alloys

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to be filled

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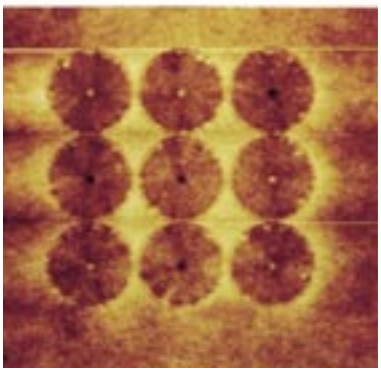
Aiming to fabricate new materials with novel properties, metallic multilayers with artificial superstructures are prepared by alternately depositing ultrathin metal layers. By using electron beam lithography technique, submicron-size wires and dots of magnetic films are fabricated. Metallic multilayers are new materials which do not exist in nature and their properties are of great interest from basic and applied points of view. The main research subjects are magnetic structures created in the metallic multilayers, which are investigated by magnetization measurements, Mössbauer spectroscopy, neutron diffraction and X-ray magnetic scattering. Magnetoresistance of magnetic domain walls is investigated with using submicron-size wires of specially designed shapes. It has been theoretically predicted that in the center of a dot with a curling magnetic structure (vortex), a spot with perpendicular magnetization should exist, but no clear experimental evidence was presented yet. Applying magnetic force microscopy to dots of permalloy with 0.1 ～ 1 micron diameter, spots of perpendicular magnetization have been observed at each center of dots. Magnetization reversal processes of the spots are investigated.



SOLID STATE CHEMISTRY II S

Advanced Inorganic Synthesis

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to be filled

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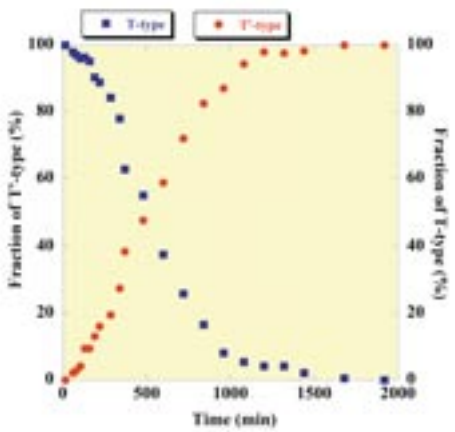
We conduct phase diagramatic studies on various complex transition metal-oxide systems and examine the chemical and thermal stability of the formed phases by means of X-ray diffraction in a wide temperature range, transmission electron microscopy, thermogravimetry, and differential thermal analysis. These studies are the most basic part of efforts toward discovering novel functional oxides. Recently we have focused on systems including high-T_C superconductors (SC) like $Bi_2Sr_2CuO_{6+\delta}$ and related phases like $Pr_{2-x}La_xCuO_4$. Investigations on $Bi_2Sr_2CuO_{6+\delta}$ have been expected to provide informations useful to elucidating the superconducting mechanism but there still remain issues to be solved concerning chemical composition, especially oxygen content, and crystal structure (modulations to be described using four dimensional space groups). To be shown below are some recent experimental results.

1) There exist at least six phases with different oxygen contents for $Bi_2Sr_2CuO_{6+\delta}$. Among these are an insulator and a SC with a T_C of 26 K, which is the highest ever reported for this series of oxides.

2) Microscopic electronic phase separation is one of the key issues concerning strongly correlated electron systems, while their chemical behaviors, including phase separations, are also quite interesting. One example is shown in the figure shown here. Peculiarly, $Pr_{2-x}La_xCuO_4$ ($1.35<x<1.5$) gradually changes its structure from the T-type to the T'-type at room temperature where ion diffusion is usually thought to be extremely slow.



Phase transformation process from T-type 214 to T'-type 214 at room temperature. Sample was obtained by quenching from 1000℃ to room temperature.

SOLID STATE CHEMISTRY IV E

Amorphous Materials

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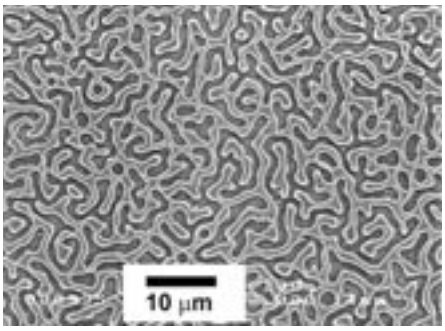
Instructor TAKAHASHI, Masahide (D Sc)
SHIMADA, Ryoko (D Sc)
Assoc Instr DORJPALAM, Enkhtuvshin

In our laboratory, we are doing studies on the preparation and characterization of new functional ceramics and amorphous materials.

1. Synthesis of novel organic-inorganic hybrid low-melting glasses: Based on the new concept, we are developing novel organic-inorganic hybrid low-melting glasses free of lead and fluorine atoms, which are environmental pollutants. In addition, we also aim at developing new optical functional low-melting glasses doped with organic substances.

2. Structural studies of glasses: For a better understanding of the functionality, analyses of the structure and electronic states of glassy materials have been conducted by means of X-ray and neutron diffraction analysis, Raman and IR spectroscopy, multinuclear high resolution solid state NMR spectroscopy, ab initio molecular orbital calculation and so on.

3. Optical functional ceramics thin films: We are trying to synthesize new functional materials with controlled nano-structure or microstructure by the sol-gel method that is known as one of the most advantageous low temperature synthesis processes. Our attention is focused especially on optical and electrical properties of these materials.



TiO_2 Thin film with two-dimensional spinodal-phase separation structure prepared by the sol-gel method

FUNDAMENTAL MATERIAL PROPERTIES I E

Molecular Rheology

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Technician OKADA, Shinichi

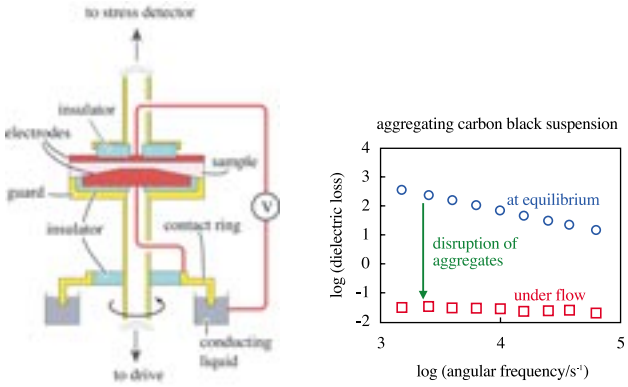
Rheology is a research field of investigating a relationship between the strain and stress of materials. How do the molecules/structures in a given material deform to raise the stress and how do they move to induce the stress relaxation ? From a molecular view summarized in these questions, this research lab combines viscoelastic, optical, scattering, and dielectric methods (see Figure) to investigate rheological properties of materials. Current research is focused on complex systems 1-4 (listed below) having various origins of the stress, and the results are to be unified for controlling the properties of supra-complex systems such as organic-inorganic hybrids.

(1) Entangled homopolymer: The stress in this material is determined by axial orientation and stretching of polymer chains. The global chain motion leading to the stress relaxation was analyzed with the above methods to demonstrate the importance of entanglement lifetime (affected by branching and length distribution of the chains) in the rheological behavior.

(2) Block copolymer: The stress in this material was found to reflect orientation/stretching of the blocks and distortions in the concentration fluctuation pattern and microdomain defects. A mechanism of flow-induced disruption of the domain alignment was related to those stress-generating mechanisms.

(3) Organic glass: The stress in this material was found to reflect the axial/planar orientation of the molecules therein as well as distortion of the molecular packing. This result was formulated as the modified stress-optical rule, thereby contributing to molecular design of low birefringence materials.

(4) Suspension of solid particles: The stress in this material results from distortion of the spatial distribution of the particles. Shear thinning of hard-core particles was attributed to saturation of this distortion while the thinning of aggregating particles was related to disruption of aggregates.



Schematic illustration of a rheo-dielectric cell and an example of measured data. Dielectric and rheological responses are simultaneously measured with this cell.

FUNDAMENTAL MATERIAL PROPERTIES II E

Polymer Materials Science

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Fundamentally important unsolved problems in polymer physics are studied using mainly scattering techniques such as neutron, X-ray and light as well as optical microscopies such as normal, polarized and confocal laser. Main subjects are (1) polymer crystallization, (2) glass transition of polymers, (3) polymer gels and (4) polyelectrolyte solutions. These studies are directed to clarify the formation processes of higher order structures of polymers and the guiding principles to control their structures. Further details are as follows:

(1) Structure formation process during the induction period of polymer crystallization is studied. Recently, polymer crystallization process under shear flow is also investigated (see Figure). (2) Frozing processes of amorphous polymers including the glass transition mechanism are studied using neutron scattering techniques. (3) Gelation processes are studied when the system involves phase separation, aiming at controlling the gel structure for applications. (4) A strongly expected phase diagram (molecular weight - concentration diagram) for polyelectrolyte solutions has been completed, particularly revealing that there exists a crystal region in the dilute regime due to strong interpolyion electrostatic repulsive forces. These forces decrease with increasing concentration and are finally screened completely to produce the swollen state just before the system becomes bulk or solid.

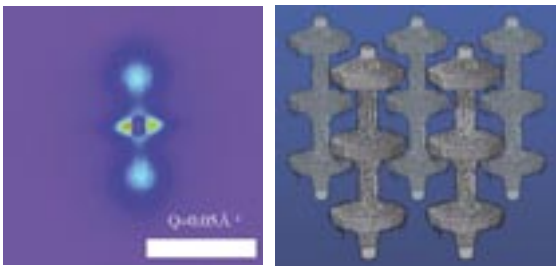

Fig: Small-angle neutron scattering pattern from elongated polyethylene fiber including ultra-high molecular weight component (left).
Right figure shows a schematic sketch of expected shish-kebab structure.

FUNDAMENTAL MATERIAL PROPERTIES III E

Molecular Dynamic Characteristics

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Molecular motion, hydrogen bonding, and structure of polymers in the different states including the liquid crystalline and molecular assembly states are studied mainly by high-resolution solid-state NMR spectroscopy, dynamic light scattering, and electron microscopy to design high-performance and high-functionality polymer materials. The major subjects are: (1) the precise characterization of slow motions ranging from 10^{-1} Hz to 10^{5} Hz for polymers by multi-dimensional solid-state NMR spectroscopy to evaluate the correlations with crystal growth, super-drawing, impact strength and so on; (2) developments of new solid-state NMR techniques to characterize the chain conformation, hydrogen bonding, and hydrophobic interactions for organic materials, and the clarification of the structure formation process in the liquid crystalline and molecular assembly states in relation to the functionality; (3) the characterization of biosynthesis, structure and assembly formation, and gelation processes for bacterial cellulose and poly(amino acid) as a model system for the structure formation and functionality realization in nature; (4) reduction of intrinsic dynamical characteristics of single chains in solution and analyses of chain dynamics and structure formations mediated between the chain architecture and the environment.

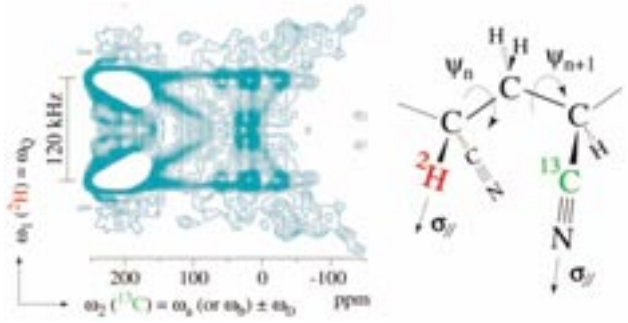

Figure
Precise analysis of the conformation of solid polyacrylonitrile by 2D solid-state heteronuclear multiple quantum coherence NMR.

ORGANIC MATERIALS CHEMISTRY I E

Polymeric Materials

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Instructor OHNO, Kohji (D Eng)
GOTO, Atsushi (D Eng)

Kinetic and mechanistic analyses are made for better understandings and systematization of the chemical and physicochemical reactions occurring in polymerization systems and for the development of better routes to the synthesis for well-defined polymers. By the application of various polymerization techniques, in particular, living radical polymerization (LRP), new well-defined polymers or polymer assemblies are prepared, and their structure/properties relationships are precisely analyzed for the development of new polymer-based materials of practical importance. Projects in progress include:

(1) Kinetics and mechanisms of living radical polymerization (LRP).

・Nitroxide-mediated polymerization (NMP), Atom transfer radical polymerization (ATRP), Reversible addition-fragmentation chain transfer (RAFT) polymerization

(2) Synthesis of new polymeric materials by living polymerizations or polymer reactions and their structure/properties studies.

・New block and random/gradient copolymers, Polymacromonomers, Polymeric derivatization of C_{60} fullerene, Homogeneous polymer gels

(3) Synthesis, properties, and applications of high-density polymer brushes.

Fabrication of High-Density Polymer Brush by Surface-initiated LRP

ORGANIC MATERIALS CHEMISTRY II E

Organic Structural Chemistry

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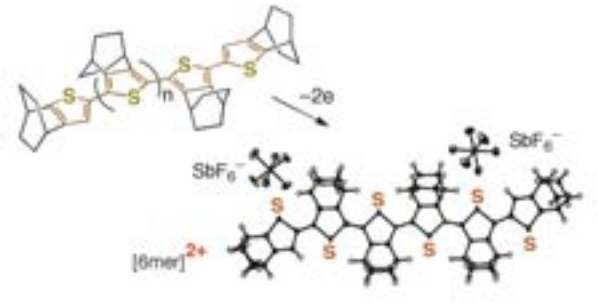
Prof KOMATSU, Koichi (D Eng)
Assoc Prof KITAGAWA, Toshikazu (D Eng)
Instructor NISHINAGA, Tohru (D Eng)
MURATA, Yasujiro (D Eng)

Synthetic, structural, and theoretical studies are being conducted on π-conjugated hydrocarbon molecules, with particular attention being paid for the redox activity. Thus, structural features are pursued to create stable cationic and radical species in order to furnish redox-active systems as fundamental models for electronic functional materials. The main subjects of the studies are as follows.

(1) Mono-and polycyclic π-conjugated systems surrounded by rigid bicyclic σ-frameworks are synthesized. These systems are characterized by the raised HOMO level due to the effective σ-π conjugation, and afford highly stabilized radical cations and even dications showing marked electrochromism. The elements such as silicon and sulfur are incorporated in these π-conjugated systems, and their electronic effects are investigated.

(2) Organic functionalization of the spherical carbon cluster, fullerene C_{60}, is conducted in order to increase the processibility and to control the electronic properties of this three-dimensional π-conjugated system. The mechanochemical solid-state reaction is applied to the structural transformation of fullerenes, particularly to the formation and characterization of dimers, C_{120} and C_{130}, and trimer, C_{180}.



Oligothiophene insulated by σ-frameworks and its dication (X-ray structure).

100% Encapsulation of hydrogen in an open-cage fullerene derivative.

SYNTHETIC ORGANIC CHEMISTRY II P

Fine Organic Synthesis

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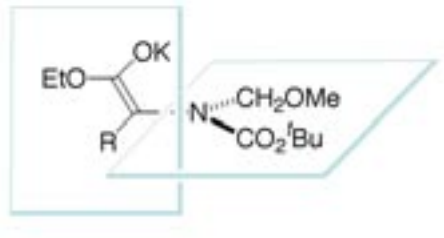
to be filled

Assoc Prof KAWABATA, Takeo (D Pharm Sc)
Instructor TSUBAKI, Kazunori (D Pharm Sc)
Technician TERADA, Tomoko

Research in this laboratory focuses on chirality, especially on the development of new methods for asymmetric synthesis and chiral molecular recognition.

(I) Asymmetric Synthesis
Studies include (1) enantioselective nucleophilic catalysis, (2) asymmetric induction based on a new concept "memory of chirality", (3) use of optically active binaphthyls for asymmetric synthesis, (4) construction of ordered secondary structure based on chirality of molecules, (5) total synthesis of biologically important natural products.
(II) Chiral Molecular Recognition.
Studies include (1) design and preparation of host molecules that change their structure by the stimuli such as light and/or guest molecules, (2) photochromic host molecules that recognize the shape and/or the length of guest molecules.
In these studies, crown ethers and hexahomooxacalix[3]arenes are employed for the capture of guest molecules.
Phenolphthalein and spiropyranes are used as chromophore. Optically active binaphtyls are used for the recognition of chirality of guest molecules.



A chiral nonracemic enolate with dynamic axial chirality. Asymmetric α-alkylation of α-amino acid derivatives proceeds *via* this intermediate in the absence of any external chiral sources.

BIOORGANIC CHEMISTRY I S

Organoelement Chemistry

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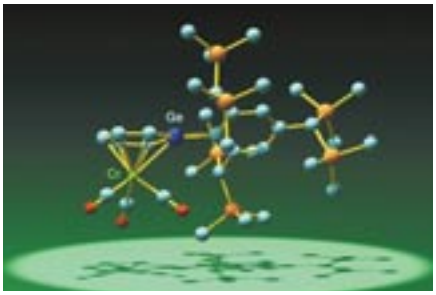
Prof TOKITOH, Norihiro (D Sc)
Assoc Prof NAKAMURA, Kaoru (D Sc)
Instructor KAWAI, Yasushi (D Sc)
TAKEDA, Nobuhiro (D Sc)
SASAMORI, Takahiro (D Sc)
Technician HIRANO, Toshiko

While organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of the "dreams" for organic chemists. In recent years, however, remarkable progress in main group chemistry has made it possible to synthesize and isolate a variety of novel compounds containing heavier main group elements. Our main research interest is the elucidation of the resemblance and difference in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting from the standpoints of not only fundamental chemistry but also opening the way to more extensive application of main group chemistry.
(1) Synthesis of Compounds Having Novel Bonding Containing Main Group Elements
We have developed novel steric protection groups, which are very useful for the kinetic stabilization of various highly reactive species of main group elements. Recently, we have succeeded in the synthesis and isolation of "novel metallaaromatic compounds containing a silicon or germanium atom [1-silanaphthalene, germabenzene, etc.]", "novel, strained ring systems containing sila- or germacyclopropane rings fused to a benzene ring [bis(silacyclopropa)benzene, germacyclopropabenzene, etc.]" and "novel doubly bonded compounds between heavier group 15 elements [phosphabismuthene etc.]" and elucidated their unique molecular structures and properties. We are now making further application of our concept to the synthesis of not only the heavier main group element compounds but also the transition metal complexes having novel structures from the viewpoints of new organoelement chemistry.
(2) Development of New Transformation Methods Using a Biocatalyst
New synthetic applications mediated by biocatalysts (microorganisms, cells of plants, and enzymes) are studied. Further extension of biocatalysts to the detoxication of environmental pollution substances is also under way.



Molecular Structure of the First Stable η^6-Germabenzene $Cr(CO)_3$ Complex

BIOORGANIC CHEMISTRY II P

Bioactive Chemistry

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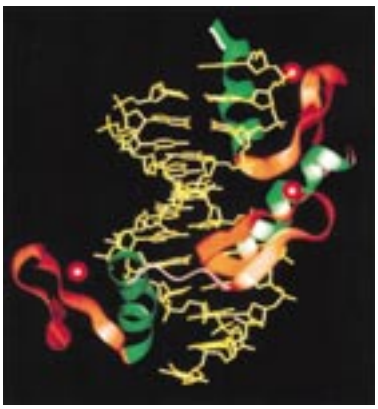
Assoc Prof FUTAKI, Shiroh (D Pharm Sc)
Instructor IMANISHI, Miki (D Pharm Sc)

As an interface of chemistry and biology, this division investigates the molecular mechanism of specific interaction between biologically active molecules and macromolecular receptors, and also aims at the design of novel functional molecules. Current research subjects are as follows:
(1) Studies on the recognition mode of nucleic acids and the regulation mechanism of genetic information by DNA binding proteins with zinc finger structure such as Sp1 and design of molecules for specific gene regulation.
(2) Design of artificial proteins with novel functions through endowing synthetic peptides with functions like an ion channel activity and consideration of the functions of natural proteins from the standpoint of non-genetic-engineering.
(3) Biochemical and biophysical studies on the mechanism of specific binding and cleavage of DNA by antitumor agents such as bleomycin, dynemicin, and C-1027.



Zinc finger protein Zif268-DNA complex

BIOORGANIC CHEMISTRY III M

Molecular Clinical Chemistry

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Prof UEDA, Kunihiro (D Med Sc)
Assoc Prof TANAKA, Seigo (D Med Sc)

Objectives of our research are elucidation of pathogenic mechanisms of cancers and neurodegenerative diseases and development of new diagnostic methods leading to prophylactic or therapeutic measures. Our current effort is focused on the followings: (1) Analysis of action of poly(ADP-ribose) synthetase (PARS) in DNA repair and the pathological significance of PARS cleavage by caspases in apoptosis. We have transfected wild or mutant PARS cDNA into PC12 or Jurkat cells to examine their effects on cell functions, particularly after exposure to apoptosis-inducing stimuli. (2) Analysis of pathogenic role(s) of PARS in ischemic diseases of heart and brain. We have developed animal models of myocardial or cerebral ischemia to analyze the distribution and activity of PARS. (3) Elucidation of physiological function of α-synuclein and its pathological role in Alzheimer's disease and Parkinson's disease. We have established, using adenovirus vector, expression systems of human wild-type and mutant α-synuclein in PC12 or rat cortical neurons to analyze their effects on neuronal function. (4) Analysis of patho-physiological roles of oncogene and antioncogene, SET and LUN, in carcinogenesis. We have cloned SET-binding protein, SEB, to elucidate their pathological roles in leukemia. We have also cloned LUN to analyze its function in association with lung cancer. (5) Development of new techniques for clinical diagnosis. We have developed IM-PCR and *in situ* PCR for gene diagnosis of viruses and tumorigenic mutations.

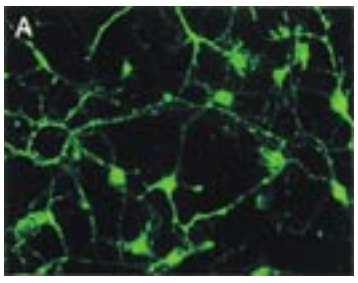

Fig.1. Primary culture of rat neuronal cells (immunostaining with anti-neurofilament antibody, x400)

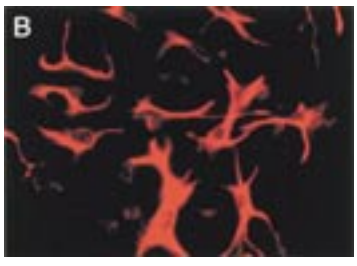

Fig.2. Primary culture of rat glial cells (immunostaining with anti-GFAP antibody, x400)

MOLECULAR BIOFUNCTION I A

Chemistry of Molecular Biocatalysts

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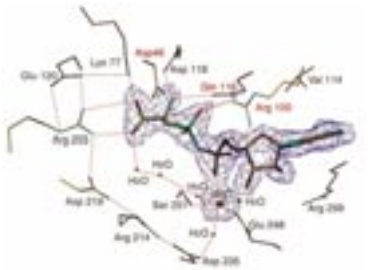
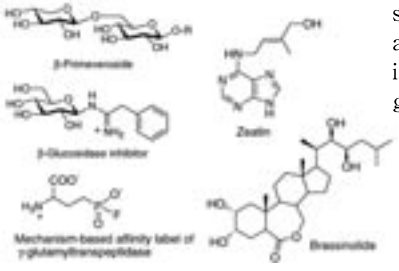
Assoc Prof HIRATAKE, Jun (D Agr)
Instructor MIZUTANI, Masaharu (D Agr)
SHIMIZU, Bun-ichi (D Agr)

Our research interest is to clarify, on molecular basis, various biological events during life cycles where many kinds of biocatalysts (enzymes) are concerned. For this purpose, we have combined and made full use of various disciplines and techniques such as natural product chemistry, organic synthetic chemistry, biochemistry, and molecular and structural biology. Our research theme covers the understanding of the physiological roles of enzymes on molecular basis, probing the reaction mechanisms and specificities of each enzymatic reaction, and the design and synthesis of new enzyme inhibitors and their applications as useful tools for enzyme study. For example, we have focussed on diglycoside-specific glycosidases such as β-primeverosidase, which is deeply concerned with the aroma formation of oolong tea and black tea, and have been studying the biocatalytic properties and the real physiological roles of this enzyme in tea plants. We have successfully developed new selective glycosidase inhibitors, β-glycosylamidines, which serve as "tailor-made" inhibitors of glycosidase according to their glycon- and aglycon-specificities. Design and syntheses of transition-state analogue inhibitors are also being pursued to understand the molecular mechanisms of ATP-dependent ligases and proteases. As a plant physiological aspect of research, we pursue the identification and understanding of the cytochrome P450 enzymes involved in the biosynthesis and catabolism of plant hormones such as brassinosteroids and cytokinins to study the activation and inactivation mechanisms of plant hormones. We also study the directed evolution of lipase to create a novel biocatalyst with unprecedented reaction specificities. The isolation and identification of hitherto unknown factors responsible for inducing resistance of sweet potato against pathogenic fungi is also under investigation.



X-Ray structure of asparagine synthetase complexed with transition-state analogy



MOLECULAR BIOFUNCTION II A

Molecular Microbial Science

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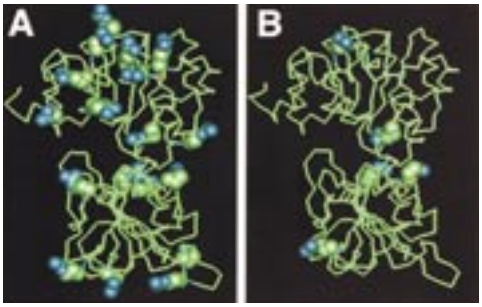
Prof ESAKI, Nobuyoshi (D Agr)
Instructor KURIHARA, Tatsuo (D Eng)
MIHARA, Hisaaki (D Agr)

Structure and function of biocatalysts are studied to elucidate the dynamic aspects of fine mechanism for their catalysis in the light of recent advances in gene technology, protein engineering and crystallography. In addition, metabolism and biofunction of trace elements are also 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 thermostable and cold-active enzymes and their application are studied. Efficient systems for the enantioselective production of various optically-active compounds have been developed with the combination of microbial enzymes. The structure and function of various hydrolases oxygenases, and oxidases are studied in order to improve their properties by protein engineering and to apply them to solving pollution problems.



Three-dimensional structures of alanine dehydrogenases from thermophilic (A) and psychrophilic (B) bacteria. The ion pairs on the molecular surface are shown as space-filling models.

MOLECULAR BIOLOGY AND INFORMATION I S

Biopolymer Structure

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Prof UMEDA, Masato (D Pharm Sc)
Instructor TAKEUCHI, Kenichi (D Pharm Sc)
KATO, Utako

We have undertaken the molecular biology, cell biology and behavioral genetics approaches to study the role of biological membrane systems, especially the principal structural element of all membranes, lipid molecules, in controlling animal morphogenesis and behavior. The membrane is a complex supramolecular complex formed by a noncovalent self-assembly of proteins, lipids and carbohydrates. Although the chemical nature and structure of the membrane are extremely diverse, the basic structure of the membrane, the lipid bilayer formed by a vast variety of lipid molecules, is shared by all forms of life.

Our long term objective is to elucidate the basic parameters that govern the molecular organization and dynamic movements of membrane lipids during cellular functions, which will provide a new insight into our understanding of the fundamental principles underlying the dynamism of complex membrane systems and 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.

Figure legend: Molecular structure of the NifS-homologous enzyme, *E. coli* CsdB

MOLECULAR BIOLOGY AND INFORMATION II S

Molecular Biology

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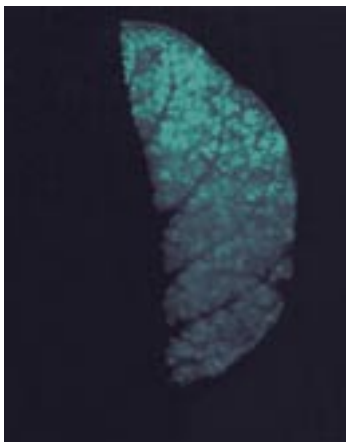
Prof OKA, Atsuhiro (D Sc)
Assoc Prof SUGISAKI, Hiroyuki (D Sc)
AOYAMA, Takashi (D Sc)
Instructor SAKAI, Hiroe (D Sc) [Suspension]
Assoc Instr OHASHI, Yohei (D Sc)
Technician YASUDA, Keiko

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 plant pathogens. Toward the goal we have been developing generally applicable procedures for understanding gene functions with transgenic plants by using *Arabidopsis thaliana* and *Agrobacterium rhizogenes*, and applying them to analyses of (i) the regulatory networks of gene expression directed by homeodomain proteins, (ii) contribution of various protein kinases and phosphatases to environmental stress responses, and (iii) genetic control of morphogenesis during leaf and flower development. Recent major results are (i) the homeodomain proteins ATHB-1, ATHB-2 and ATHB-10 concern morphogenesis during leaf development, shade avoidance, and morphogenesis of trichome cells, respectively; (ii) the bacterial-type response regulators are involved in phytohormone responses in higher plants; (iii) combinations of the MADS box proteins are essential for development of the flower organs; and (iv) the entire genome structure of the hairy-root-inducing plasmid carried by *A. rhizogenes* A4 has been determined.



A transgenic tobacco leaf in which the firefly luciferase gene was made inducible by exogenous steroid hormones; the right half of leaf was sprayed with a hormone.

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE I E

Organic Main Group Chemistry

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Prof TAMAO, Kohei (D Eng)
Instructor TSUJI, Hayato (D Eng)
SAEKI, Tomoyuki (D Eng)

Our research interests encompass the elements science, molecular science, and materials science. Current research projects are concerned with the development and application of new functional organic compounds of the main group elements such as silicon, boron and others, and of new synthetic methodologies based on transition metal catalyzed reactions. The main subjects are as follows.
(1) Conformation-controlled oligosilanes and polysilanes for full-understanding of the sigma-conjugation.
(2) Construction of some donor-oligosilane-acceptor frameworks and their charge-transporting ability.
(3) Construction and photophysical properties of novel one-dimensional linear sigma-pi conjugated system.
(4) New carbon-carbon bond forming reactions catalyzed by transition metal complexes for construction of pi-conjugated monomers and polymers containing main group elements.

Silicon-Containing sigma-Conjugated Systems

Conformation-Controlled Oligosilanes and Their Photophysics

Silicon-Containing pi-Conjugated Systems

An Efficient Electron-Transporting Material
for Application to Organic EL Devices

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE II S

Advanced Solid State Chemistry

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Assoc Prof TERASHIMA, Takahito (D Sc)
Instructor AZUMA, Masaki (D Sc)
Assoc Instr YAMAMOTO, Shinpei (D Eng)

We are searching for new 3d-transition metal oxides and their new functions by controlling three important chemical parameters which are composition, structure, and morphology. For this purpose we conduct high-pressure synthesis (up to 10GPa and 1500℃), film growth (pulsed laser ablation), and microscopic fabrication.
In the focus of our interest are Fe^{4+}- and Ni^{3+}- oxides like $SrFeO_3$ showing properties dominated by oxygen p-hole character, Bi-3dtransition metal oxides where magnetism and ferroelectricity coexist, cupric oxides suitable for experiments to clarify the mechanism of high-T_c superconductivity like $(Ca,Na)_2CuO_2Cl_2$, $SrCu_2O_3$ (two-legged ladder), and $Sr_2Cu_3O_5$ (three-legged ladder), manganese oxides showing colossal magnetoresistance,.
The most remarkable technical progress about the high-pressure synthesis is of single crystal growth. Shown in the figure are the crystals grown at 3 to 4.5 Gpa and 1300℃.
Concerning thin films, light emission from a specific high-T_c p-i-n junction and other transition metal oxides are being investigated.

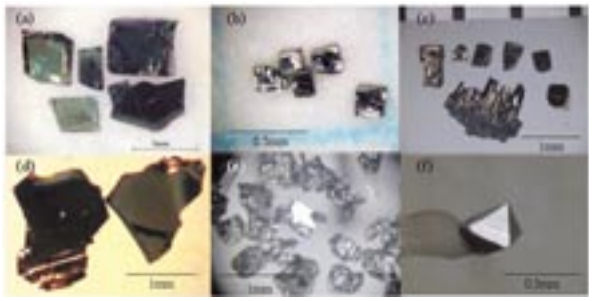

Fig.1 : Single crystals of (a) $(VO)_2P_2O_7$、(b) $BiMnO_3$、(c) $PrNiO_3$、(d) $Ca_{1.9}Na_{0.1}CuO_2Cl_2$、(e) $CaFeO_3$、(f) $Tl_2Ru_2O_7$ grown at 3～4.5GPa and 1300℃

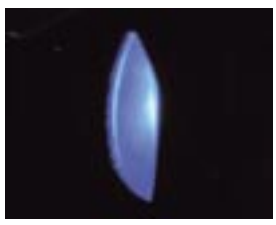

Fig.2 : Blue light emission from an oxygen-deficient $SrTiO_3$ single crystal.

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE Ⅲ E

Organotransition Metal Chemistry

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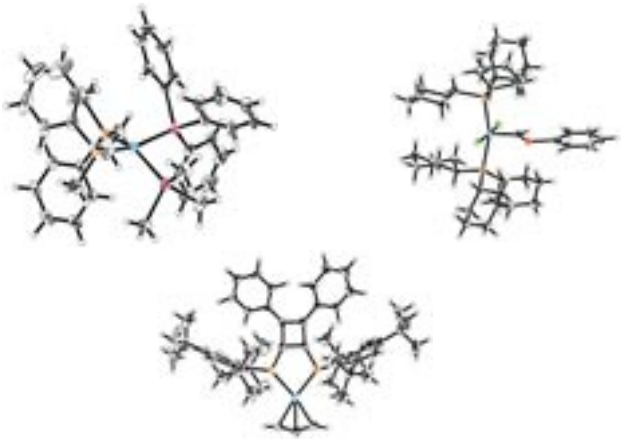
Prof OZAWA, Fumiyuki (D Eng)
Instructor KATAYAMA, Hiroyuki (D Eng)

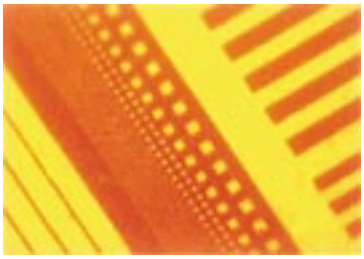
This is a new research laboratory launched in the 2003 academic year, aiming at establishment of new efficient synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry.

New concepts and ideas of well-defined 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 ligands and their complexes for new catalysis, and (2) synthesis and catalytic properties of a series of transition metal–heavy element complexes.



X-Ray structures of transition metal catalysts

The above studies allow us to develop highly efficient ways of constructing functional organic molecules. A particular interest is focused on the synthesis of pi-conjugated polymers with well-defined structures, which exhibit novel optical properties.



Optical image of micropatterned light-emitting material

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE Ⅳ S

Photonic Elements Science

Tel : Pending Fax : Pending
e-mail : Pending

to be filled

(Prof : to be filled in December)

This is a new research laboratory launched in the 2003 academic year, aiming at the development and establishment of optonanoscience for creation of innovative functional materials.

BIOINFORMATICS CENTER S

Bioknowledge Systems

Tel : 0774-38-3270 Fax : 0774-38-3269
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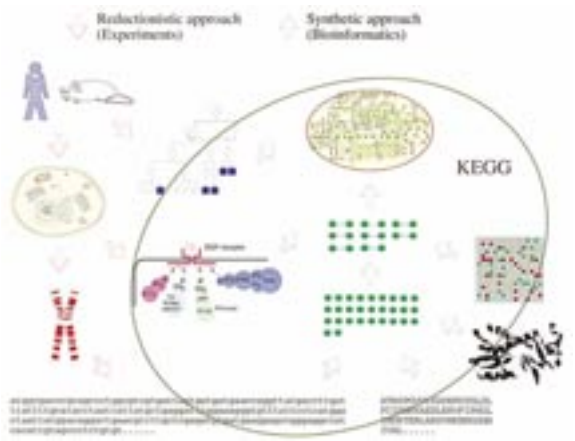
Prof KANEHISA, Minoru (D Sc)
Assoc Prof GOTO, Susumu (D Eng)
Instructor KAWASHIMA, Shuichi
Visiting Instructor OKUNO, Yasushi (D Pharm Sc)

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. However complete, such experimentally determined catalogs of genes, RNAs, and proteins only tell us about the building blocks of life. They do not tell us much about how life operates as a system, such as systemic functional behaviors of the cell or the organism.

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, of the biological systems by analyzing complex interactions among building blocks and with dynamic environments. We have been developing such bioinformatics technologies and the KEGG system, which is our attempt to uncover and utilize cellular functions through reconstruction of protein interaction networks from the genome information. We are also responsible for the development and operation of the GenomeNet database service (http://www.genome.jp/).



BIOINFORMATICS CENTER I

Biological Information Network

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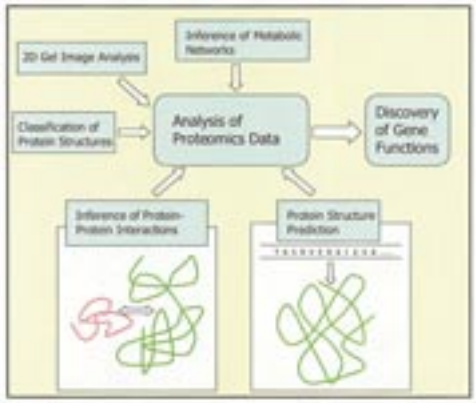
Prof AKUTSU, Tatsuya (D Eng)
Instructor UEDA, Nobuhisa (D Eng)

Due to rapid progress of the genome projects, whole genome sequences of many organisms and a draft of human genome sequence have already been determined. But, the determination of the whole genome sequence does not mean the end of analysis of the genetic code. We need to understand the meaning behind the genetic code. For this purpose, we need advanced information technologies that can be applied to large amounts of heterogeneous information. In particular, technologies for analyzing proteomics data are important in order to understand the functions of genes. We develop algorithms and software tools for analyzing proteomics data based on advanced information technologies such as artificial intelligence, theory of algorithms and machine learning. Application areas include protein structure prediction, classification of protein structures, inference of protein-protein/protein-ligand interactions, inference of genetic/metabolic networks and image analysis of 2D electrophoresis gels.



BIOINFORMATICS CENTER

Pathway Engineering

Tel : Pending Fax : Pending
e-mail : Pending

This laboratory aims at developing a theory on the stability of a system against perturbations and applying the theory to practice such as the drug discovery. The perturbations in this context are, for example, mutations in genes and environmental changes in the system of life that cause genetic and environmental diseases. It is important to consider what kind of (counter) perturbation, e.g. a combination of drugs, is necessary to stabilize the system when we find a relationship between a disease and mutations in several genes, the original perturbations that destabilize the system. We should treat an organism or a cell as a system and construct a knowledge base of biological and medical information about regulation of genes, cells and metabolisms to simulate the stability in the system. We consider the system as a collection of metabolic and other pathways in the pathway engineering and mainly study on the following three topics.

1. Design of metabolic pathways based on genomic and chemical information,
2. Theoretical approach to stability of pathways against perturbation such as mutations in a genome and environmental changes, and
3. Practical application of the theories on pathway stabilities.

CONTRIBUTED CHAIR

Proteome Informatics (SGI Japan)

Tel : 0774-31-4901 Fax : 0774-31-4904
e-mail : bic4@kuicr.kyoto-u.ac.jp

Visiting Assoc Prof MAMITSUKA, Hiroshi (D Sc)
Visiting Instructor YAMAGUCHI, Atsuko

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

BIOINFORMATICS CENTER

Bioinformatics Training Unit

Tel : 0774-38-3902 Fax : 0774-38-3059
e-mail : toh@kuicr.kyoto-u.ac.jp

Visiting Prof TOH, Hiroyuki (D Sc)
Visiting Assoc Prof KUMA, Keiichi (D Sc)
Visiting Instructor DAIYASU, Hiromi (D Sc)
ICHIHARA, Hisako

Evolutionary studies based on molecular biology are called "molecular evolutionary biology". Living organisms have acquired a 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. In addition, 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 molecular biological data including sequence and structure data of genes and proteins, genome data, and expression profile data. We also analyze such data from the evolutionary viewpoint, to obtain novel biological knowledge. We are now investigating genome comparison, molecular evolution of archaebacteria, functional analysis of GPCR, protein structure comparison, improvement of evolutionary trace method, glycobiology, and inference of gene expression network from expression profile data. Our protein structure comparison programs are available at a web site, ASH (Alignment of Structural Homologues) (http://timpani.genome.ad.jp/~ ash/).

NUCLEAR SCIENCE RESEARCH FACILITY S

Particle and Photon Beams

Tel : 0774-38-3281 Fax : 0774-38-3289
e-mail : noda@kyticr.kuicr.kyoto-u.ac.jp

Prof NODA, Akira (D Sc)
Assoc Prof IWASHITA, Yoshihisa (D Sc)
Instructor SHIRAI, Toshiyuki
Technician TONGU, Hiromu

Charged particle and photon beam generated with accelerators and their instrumentation both for fundamental research and practical applications are scope of our research. The main subjects are: beam dynamics in high intensity accelerators: beam handling during injection and extraction processes at the accelerator ring, beam diagnosis in accelerators: radiation mechanism of photons from an electron storage ring: development of a compact accelerator dedicated for cancer therapy: and irradiation of materials with charged particle and photon beams. Details are given below for main items.

(1) Control of the beam divergence due to space charge effect of the charged particles: Beam as an assembly of charged particles diverges because of Coulomb repulsive force, which is more remarkable at lower energies. Ion optics to suppress this effect and enables the beam transport of high current without emittance growth has been studied.

(2) Radiation process of electron beam: An electron storage ring, KSR with circumference and the maximum energy of 25m and 300 MeV, respectively, has been constructed as a light source in VUV and soft X-ray region. In addition, KSR is also utilized as a pulse stretcher of the 100 MeV electron linac to enlarge its duty factor, which will leads to improvement of efficiency and precision of experiments.

(3) Realization of a compact ion accelerator dedicated for cancer therapy: Charged particle cancer therapy is recently considered to be very promising because it is free from damage of function and shape of human body caused by surgery operation. In order to develop a machine with reasonable size suited for a hospital as a regional center, a compact ion synchrotron has been developed.

Layout of the Electron Accelerator, KSR

Beams and Fundamental Reaction

Tel : 0774-38-3291(SAKABE)/3286(MATSUKI) Fax : 0774-38-3289
e-mail : sakabe@kyticr.kuicr.kyoto-u.ac.jp
matsuki@carrack.kuicr.kyoto-u.ac.jp

Prof
SAKABE, Shuji (D Eng)-L-
MATSUKI, Seishi (D Sc)-R-
Instructor
HASHIDA, Masaki (D Eng)

We have two groups in this division.
(1) Laser-matter interaction science
Physics of matter in intense optical field created by powerful lasers is studied. The main subjects are ultra-intense femtosecond laser technology, laser-matter interactions and their applications. Intense short pulse laser interaction with solid surface and its application to laser superfine (nano) material processing is studied. With much more intense short pulse lasers, ionization and Coulomb explosion of large molecules, clusters, and micro-particles and high energy radiation (x-ray, electrons, ions) generation in plasmas are of our interest to promote a new field of laser nuclear science. Main facility is the T^6-laser (10TW, 100fs) available since 2003.

(2) Astroparticle physics
Quest for the origin of dark matter in the Universe is one of the most important subjects in astro- and particle physics. Axion, invoked to solve the so called "Strong CP problem" in the QCD theory, is suggested to be an elegant solution for the dark matter problem in the Universe. The main subjects of research here are to search for dark matter axions with Rydberg atoms in a microwave cavity at low temperature and strong magnetic-field environment, and to investigate its related physics of high Rydberg atoms in an external electromagnetic field. Also applications of Rydberg atoms in a cavity to fundamental research such as quantum information processes are being studied.

SOLID STATE CHEMISTRY

Visiting Prof **INOUE, Junichiro (D Eng)**
(Graduate School of Technology, Nagoya University)

Visiting Assoc Prof **YAMANAKA, Akio (D Sc)**
(Faculty of Photonics Science and Technology
Chitose Institute of Science and Technology)
[Promoted on 1 April 2003]

Prof. Inoue theoretically studies magnetism and superconductivity based on the electron theory of solids in order to find and elucidate novel quantum phenomena in solids. The main subjects in progress are (1) transport properties of nanoscale magnets, superconductors, and magnetic/superconducting junctions, and (2) physical phenomena caused by the strong electron-correlation in transition-metal oxides.
The research interests of Associate Prof. Yamanaka broadly lie in the physics of new materials, including superconductors, semiconductor quantum dots, glass, incipient ferroelectricity of oxides and phosphor materials. He also studies hyper-Raman spectroscopy and its application.

SYNTHETIC ORGANIC CHEMISTRY

Visiting Assoc Prof **SUGIO, Naritoshi (D Pharm Sc)**
(Senior Research Associate, Science & Technology
Office, Yokohama Center, Mitsubishi Chemical Co.,Ltd.)
(Group Manager, Research & Development Center,
ZOEGENE Co.,Ltd.)

Dr. Sugio has probed the relationships between structure and function in various enzymes of biological importance by means of X-ray crystallography. He has developed also various new techniques to obtain supreme crystals of proteins for high-resolution analysis by exploiting crystallization in space.

FUNDAMENTAL MATERIAL PROPERTIES

Visiting Prof **YABUKI, Kazuyuki (D Eng)**
(Toyobo Co., Ltd. General Manager of Tsuruga Center)

Visiting Assoc Prof **SATO, Takaya (D Eng)**
(Nisshinbo Industries Inc. R&D Center Chief Scientist)

The major research subjects in this subdivision are as follows:
(1) Investigations on developments of high-tenacity and high-modulus materials are fundamentally and industrially important also from an ecological and energetic point of view. Although some high-performance materials overcoming steel have already been developed for flexible or rigid polymers by respectively employing gel-spinning/superdrawing or liquid crystal spinning, their tenacities are still levels of 1/5 - 1/10 compared to the ultimate tenacity theoretically assumed. In this subject, the causes are clarified by precisely analyzing the structure and dynamics in the structure formation process by solid-state NMR and high-power X-ray diffraction methods and further developments of higher-performance polymer materials will be made.
(2) "Precision Polymerization of Ionic-Liquid Monomers": Ionic liquids are a new class of materials that are characterized by high degrees of ionic conductivity, inflammability, and chemical/physical stability. This project attempts to develop new functional nano-scaled materials on the basis of precision radical polymerization of monomers with ionic-liquid side-chains.

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

Visiting Prof **TATSUMI, Kazuyuki (D Eng)**
(Research Center for Materials Science, Nagoya University)

Visiting Assoc Prof **YANO, Yoshihiko (D Eng)**
(TDK Co., Ltd., Research & Development Center)

The research project of Prof. Tatsumi aims at the creation and analysis of new dynamic complexes in the interdisciplinary field of transition metal and heavy main group elements. Research subjects include (1) Synthesis and reactions of electron-deficient transition metal chalcogenides, (2) artificial construction of an active site of reductive metal enzyme clusters, and (3) theoretical studies on electronic state and reactivity of transition metal complexes.
The research project of Associate Prof. Yano aims the fabrication of new functional devices using thin-film materials. Research subjects include (1) fabrication of color inorganic EL (iEL) displays based on the two remarkable technologies, a blue emitting phosphor, $BaAl_2S_4$:Eu and a thick-film, high-K dielectric structure and (2) an ultra-high density memory using AFM technology.

Visiting Prof Liu, Yunqi (D Eng)

(Professor: Institute of Chemistry, Chinese Academy of Sciences, P.R. China)
[Term of Visit : January 5 , 2004 - April 4 , 2004]

Prof. Liu's research interests encompass a wide range of materials science from organic synthesis to semi-conductor devise technology. In particular, his group has contributed to the organic synthesis of phthalocyanines, porphyrines, and pi-conjugated polymers, the thin-film preparation by LB self-assembly method, vacuum deposition, and spin casting method, the fabrication of devises and analysis of their performance such as light-emitting diodes, field-effective transistors, non-linear optical materials, gas sensors, electrochromic materials, and photochromic materials, and the development of innovative method for the synthesis of carbon nanotube and the finding of its amphiphobic properties for unique application. Prof. Liu, as the visiting professor, will extend some of these researches from the view point of elements science, and start some collaborative studies with researchers in our institute.

Nobel Prize

(period of one's tenure of ICR)

YUKAWA, Hideki	1949	Physics	(1943～1968)

Order of Culture

YUKAWA, Hideki	1943	Atomic Physics	(1943～1968)
HAYAISHI, Osamu	1972	Biochemistry	(1959～1976)
SAKURADA, Ichiro	1977	Polymer	(1936～1967)
MITSUDA, Hisateru	1994	Food Science	(1955)

Persons of Cultural Merits

YUKAWA, Hideki	1951	Atomic Physics	(1943～1968)
HORIBA, Shinkichi	1966	Physical Chemistry	(1927～1947)
HAYAISHI, Osamu	1972	Biochemistry	(1959～1976)
SAKURADA, Ichiro	1977	Polymer	(1936～1967)
MITSUDA, Hisateru	1989	Nutrition, Food Science	(1955)
HORIO, Masao	1993	Polymer, Materials	(1955～1970)

The Japan Academy Prize

SASAKI, Nobuji	1944	(1942～1959)
SAKURADA, Ichiro	1955	(1936～1967)
INOUE, Yoshiyuki	1959	(1943～1959)
KIMURA, Ren	1959	(1939～1956)
KATAGIRI, Hideo	1960	(1942～1960)
HAYAISHI, Osamu	1967	(1959～1976)
SUZUKI, Tomoji	1979	(1957～1965)
MITSUDA, Hisateru	1980	(1955)

Medal of Honor with Purple Ribbon

SAKURADA, Ichiro	1956	(1936～1967)
TAKEI, Sankichi	1961	(1937～1959)
ODA, Ryohei	1972	(1955～1970)
SUITO, Eiji	1977	(1951～1975)
TAKADA, Toshio	1987	(1963～1986)
SAKKA, Sumio	1996	(1953～72/1983～94)
SODA, Kenji	1997	(1965～1996)
SHINJO, Teruya	2000	(1966～2002)

Research Buildings

①Main Building

⑩Accelerator Laboratory

④High– resolution spectromicroscope Laboratory

Drainage Monitor Center of Uji Campus

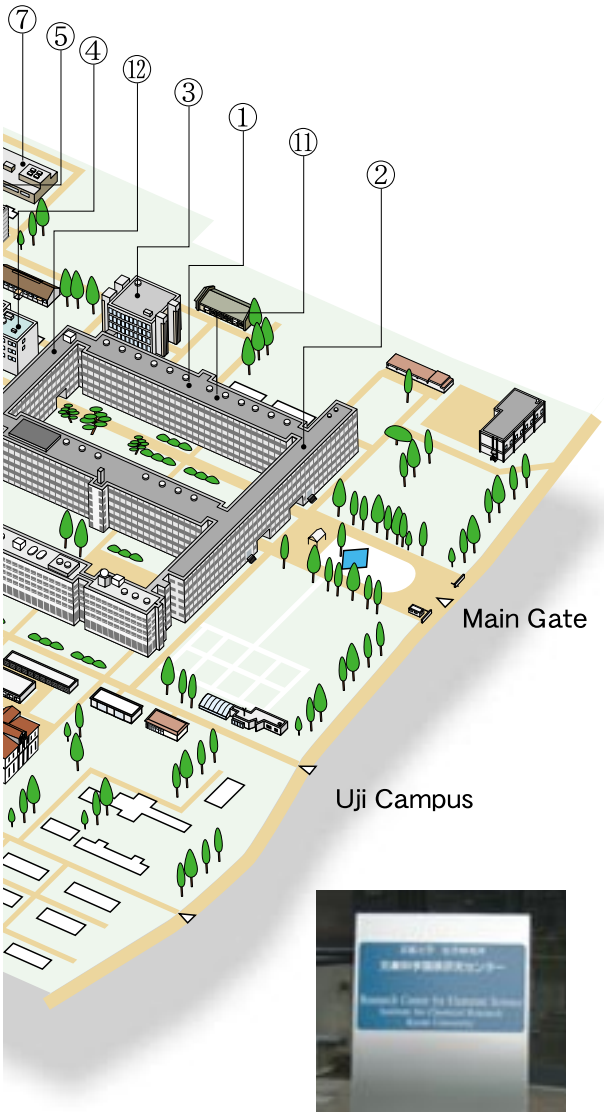
Institute for Chemical Research

Campus Area	216,938 ㎡
Buildings (Total area)	22,013 ㎡
①Main Building & Annex	12,969 ㎡
②Administration Office (3rd.Fl.)	
③Joint Research Laboratory	3,705 ㎡
④High-Resolution Electron Spectromicroscope Laboratory	913 ㎡
⑤Low-Temperature High-Resolution Electron Microscope Laboratory	586 ㎡
⑥Low-Temperature Laboratory	760 ㎡
⑦Bioengineering Laboratory	540 ㎡
⑧Bioinformatics Center	496 ㎡
⑨Nucleic Acids Laboratory	1,207 ㎡
⑩Acceterator Laboratory, Nuclear Science Research Facility	2,668 ㎡
⑪International Research Center for Elements Science	
⑫Uji Library, Kyoto University	

Uji Campus is located at the verdurous riverfront of the Uji River. Here has been a strategic point between Kyoto and Nara, the old capitals of Japan, and there are many historical heritages such as the Obaku-san Manpukuji Temple that was a center of the advanced culture and arts introduced from Ming. We endeavor to enrich the buildings and facilities those are suitable to the center for the most advanced studies and harmonious with nature and the a local community.

⑧Bioinformatics Center

⑨Nucleic Acids Laboratory



⑦Biotechnology Laboratory

⑪International Research Center for Elements Science

③Joint Research Laboratory

Major Research Instruments

Electron Spin Resonance Spectrometer

Electron Storage Ring KSR

Pulsed Laser Deposition System

Solid-State NMR Spectrometer

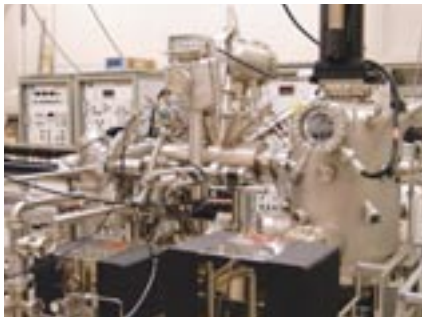
Computational Chemistry and Bioinformatics Servers (SGI Origin 3800 supercomputer systems)

The Institute's Supercomputer Laboratory houses SGI Origin 3800 supercomputer systems (left) and SUN Fire 15K server systems (below), which are used for research in computational chemistry and bioinformatics as well as for the GenomeNet Service.

GenomeNet Server(SUN Fire 15K server systems)

High-Pressure Synthesis Apparatus

Multi-Purpose Automatic Bioreactor



Photoemission Spectrometer

P3-Level Pecombinant DNA Technology Laboratory

Low-Temperature Laboratory (Helium Liquifier)

New Materials Development Laboratory

High Resolution Electron Spectro-Microscope

This is one of the highest performance microscopes in the world with accelerating voltage of 1,000 kV, maximum magnification of 6,000,000 and spatial resolution of 0.12 nm. Imaging plate is employed as a high quality detector in addition to photo-films and CCD camera. By using an electron energy spectrometer, inelastically scattered electrons can be analyzed and re-imaged so as to reveal elemental distribution in a specimen. The detectable mass reaches to less than 10-20 g. A phthalocyanine molecule was directly imaged in atomic resolution.

MALDI-TOF Mass Spectrometer

This matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometer can be used not only for biopolymers, including proteins, nucleic acids, sugars, and lipids, but also for synthetic polymers and organic molecules. This apparatus is particularly useful for the structural characterization of the large and complex molecules which cannot be attained by any other means such as the NMR spectroscopy.

600 MHz NMR Spectrometer

One- and two-dimensional solution spectra and relaxation properties including diffusion can be measured with high resolution for such nuclei as ^{1}H, ^{13}C, ^{14}N, ^{15}N, ^{17}O, ^{19}F, ^{31}P, and metallic elements. Most of these elements are relevant to today's issues in biochemistry, chemistry, and physics. The NMR machine is useful and powerful for a variety of measurements, because it is equipped with computer-controlled field-gradient probes and because it is connected to other NMR machines in our institute by a network system. The equipment is applied for the physico-chemical study of water and aqueous solutions under ambient supercritical conditions.

X-ray Crystallographic Diffration System with 2-Dimensional Detector

Staff and Students

University Staff

(As of September 1, 2003)

Professor	Associate Professor	Instructor	Sub-total	Associate Instructor	Technician	Part Timer	Sub-total	Grand Total
28 (3)	19 (4)	43	90 (7)	5	10	88	103	193 (7)

Numbers in parentheses represent visiting Professors

Graduate Students

(As of May 1, 2003)

Classification		1999	2000	2001	2002	2003
Science	Master's Course	40	43 (1)	57 (1)	47	36 (1)
	Doctoral Course	61 (5)	55 (4)	45 (6)	40 (3)	52 (3)
Engineering	Master's Course	33	33	38 (2)	38 (2)	31
	Doctoral Course	30 (2)	26 (3)	24 (2)	23 (5)	25 (8)
Agriculture	Master's Course	17 (2)	17 (1)	21	24	24
	Doctoral Course	9 (2)	8 (3)	9 (5)	13 (4)	11 (3)
Pharmaceutical Sciences	Master's Course	15	16	16	14	18 (1)
	Doctoral Course	6 (1)	9	9 (1)	10	8
Medicine	Master's Course	0	0	0	0	0
	Doctoral Course	3 (2)	4 (3)	3 (2)	2 (2)	1 (1)
Informatics	Master's Course	—	—	—	6 (2)	1 (1)
	Doctoral Course	—	—	—	1	5 (1)
Total	Master's Course	105 (2)	109 (2)	132 (3)	129 (4)	110 (3)
	Doctoral Course	109 (12)	102 (13)	90 (16)	89 (14)	102 (16)
Total		214 (14)	211 (15)	222 (19)	218 (18)	212 (19)

Figures in parentheses represent the number of foreign students

Origins of Graduate Students

(As of May 1, 2003)

University		Master's Course	Doctoral Course	Sub-Total
Domestic	Kyoto University	56	39	95
	Other Universities	51	47	98
Sub-Total		107	86	193

	Country	Master's Course	Doctoral Course	Sub-Total
Foreign	China, P. R.	2	3	5
	Indonesia	1	1	2
	Korea, R.		7	7
	Mongolia		1	1
	Morocco		1	1
	Nepal		1	1
	Thailand		2	2
Sub-Total		3	16	19
Total		110	102	212

Other Research Students, Fellows and Associates

(As of May 1, 2003)

	Research Student	Research Fellow	Postdoctral Fellow of JSPS	Other Research Associate	Total
1999	6	4	2	9	21
2000	16	5	7	13	41
2001	8	4	8	7	27
2002	7	1	3	9	20
2003	5	2	6	8	21

Figures of JSPS fellows (PD) represent the number of newly adopted

Finances

(ten thousands yen)

	Personel	Non-Personel	Grants-in-Aid for Scientific Research	Partnership between Universities and Industry	Other※4 Funds	Donation for Research	Total
1998	1,478,309	1,432,749	691,782	121,523	—	65,520	3,789,883
1999	1,310,127	1,284,260	488,921	134,470	—	73,860	3,291,638
2000	1,407,951	1,549,215	954,280	418,314※1	—	78,062	4,407,822
2001	1,397,585	1,725,272	795,105	356,231※2	98,673	106,478	4,479,344
2002	1,471,582	1,680,788	652,900	130,578※3	514,748	109,766	4,560,362

※1For 2000, including other competitive research funds of the Japanese Government (308,796)
※2For 2001, including other competitive research funds of the Japanese Government (315,230)
※3For 2002, including other competitive research funds of the Japanese Government (17,998)
※4Until 2000, "Other Funds" were included in the funds of Partnership between Universities and Industry

Major Grants and Funds in 2002

Grants-in-Aid for Scientific Research (over ten million yen)

Specially Promoted Research (2)/
- Elements Science: Construction of Organic and Inorganic Frameworks Focusing on Quality of Elements — TAMAO, Kohei
- Search for Dark Matter Axions — MATSUKI, Seishi

Priority Areas Research (2)/
- Role of Polymers for Constructing all Solid-state Ionic Devices — KOHJIYA, Shinzo
- A Study on the Spatial Inhomogeneity of Spin- and Charge-Density in Transition Metal Oxides — YAMADA, Kazuyoshi
- Construction and Retrieval of Highly Integrated Biological Databases — GOTO, Susumu
- Construction and Characterization of Composite Bioctalysts — ESAKI, Nobuyoshi

Scientific Research (A) (1)/
- Superstrong Permanent Magnet Quadrupole for Final Focus Lens of Linear Collider — IWASHITA, Yoshihisa

Scientific Research (A) (2)/
- Elucidation of Photochemical Reactivity in Glass-an Approach from Electronic and Vibrational Structures- — YOKO, Toshinobu
- Studies on the Syntheses of Novel Aromatic Species Containing a Heavier Group 14 Element and Their Structures, Properties and Functions — TOKITOH, Norihiro
- Science and Functions of Ultra-Densely Polymer Grafted Solid Surfaces — FUKUDA, Takeshi
- Searches for New 3d Transition Metal Oxides Dominated by Oxygen p-Hole Character — TAKANO, Mikio

Scientific Research (B) (2)/
- Development of Novel Systems for the Detection of Intracellular Protein Interaction Using Membrane-permeable Peptides — FUTAKI, Shiroh

Grant-in-Aid for Young Scientists (A) (The Ministry of Education, Culture, Sports, Science and Technology of Japan)/
- Bioconversion of Fluorinated Organic Compounds: Mechanistic Enzymology of Fluorination and Defluorination and Application — KURIHARA, Tatsuo

Partnership between Universities and Industry (over ten million yen)

Contact Research
Ministry of Public Manegement, Home, Affairs, Posts and Telecommunucatuins/
- Study on Optical Devices Using Novel Organic/Inorganic Hybrid Low-melting Glasses — SHIMADA, Ryoko

MEXT Research Revolution 2002 (RR2002)
Nanotechnology Support Project of MEXT, Japan/
- Precise Analysis Support of Nanosize Materials — ISODA, Seiji

Protein3000/
- Structural Genomics Consortium for Research on Protein Higher-Order Structure Formation System; Principal Investigator: Prof. Kunio Miki, Graduate School of Science, Kyoto University — HATA, Yasuo
- Structural Genome for Intracellular Signal Transduction: Principal Investigator : Prof. Inagaki Fuyuhiko, Graduate School of Pharmaceutical Sciences, Hokkaido University — TOH, Hiroyuki

Other Funds (over ten million yen)

Special Coordination Fund of the Ministry of Education, Culture, Sports, Science, and Technology of Japan/
- Hierarchy of Transcriptional Controls in Plant Signal Transduction — OKA, Atsuhiro
- Computational and Experimental Analysis for Reconstruction of Genetic and Molecular Networks — KANEHISA, Minoru
- Bioinformatics Training Unit — KANEHISA, Minoru

JSPS Research for the Future Program/
- Biological Systems Database (KEGG) and Genome Information Science — KANEHISA, Minoru

Industrial Technology Research Grant Program by New Energy and Industrial Technology Development Organization (NEDO) of Japan/
- Control of Higher Order Structures of Polymer Materials by a Rapid Temperature Jump Method — NISHIDA, Koji
- Production of Useful Compounds and Environmental Purification by Cryobiotechnology with Cold-adapted Microorganisms — KURIHARA, Tatsuo

Research Activities

Publications

1997	1998	1999	2000	2001	2002
397	430	465	390	407	497

Visitors from foreign countries in 2002

84 people from 18 countries

ICR International Symposiums

1st November 7-8, 1996
The First ICR International Symposium-Controlled Organization and Molecular Dynamics of Polymers; Uji, Kyoto

2nd August 4-8, 1997
15th International Colloquium on Magnetic Films and Surfaces (ICMFS'97); Queensland, Australia

3rd May 29-31, 1999
The 12th International Symposium on Organosilicon Chemisty; Kyoto

4th July 29-30 , 1999
XVIth International Seminar on Ion-Atom Collisions (ISIAC XVI) ; Uji, Kyoto

5th March 5-8, 2002
17th International Colloquium on Magnetic Films and Surfaces; Kyoto

6th January 31- February 1, 2002
The Science and Technology of Polymer Assembly:
The Global Strategy in 21st Century; Uji, Kyoto

7th August 19-20 , 2002
International Seminar on Photoionization in Atom; Uji, Kyoto

8th April 2-4 , 2003
9th International Seminar on Elastomers; Kyoto

Awards

(the last 8 years)

1996	TSUJI, Masaki	The Society of Fiber Science and Technology, Japan Prize for Excellence in Fiber Research
	YOSHIMURA, Tohru	The Morinaga Hoshi-kai Award
1997	SHINJO, Teruya	The Magnetics Society of Japan Award
	TAKANO, Mikio	Society of Non-Traditional Technology, The Superconductivity Science and Technology Award
	TERASHIMA, Takahito	Society of Non-Traditional Technology, The Superconductivity Science and Technology Award
	FUTAKI, Shiroh	The Japanese Peptide Society Award for Young Scientists
1998	MIBU, Ko	The Magnetics Society of Japan Young Researchers of the Year (Takei Award)
	HIRAI, Asako	The Cellulose Society of Japan Award
	KOMATSU, Koichi	The Divisional Award of The Chemical Society of Japan
	FUJI, Kaoru	The Pharmaceutical Society of Japan Award
	TOKITOH, Norihiro	Japan IBM Science Award
	FUTAKI, Shiroh	The Pharmaceutical Society of Japan Award for Young Scientists
	UEDA, Kunihiro	Shibata Susumu Memorial Award of the Clinical Pathology Research Foundation
1999	MORIGUCHI, Sakumi	The Japanese Society for Electron Microscopy, Award for the Outstanding Technologist
	KAJI, Hironori	Award for Encouragement of Research in Polymer Science, The Society of Polymer Science, Japan
	TAMAO, Kohei	The Chemical Society of Japan Award
	YAMAGUCHI, Shigehiro	The Society of Silicon Chemistry, Japan Award for Young Chemists
	HIRATAKE, Jun	The Japan Bioscience, Biotechnology, and Agrochemistry Society Award for the Encouragement of Young Scientists
	AKUTSU, Tatsuya	Japanese Society for Artificial Intelligence Research Promotion Award
	MIYANO, Satoru	Japanese Society for Artificial Intelligence Research Promotion Award
2000	SHINJO, Teruya	Medal of Honor with Purple Ribbon
	URAYAMA, Kenji	Award for Encouragement of Research in Polymer Science, The Society of Polymer Science, Japan
	INOUE, Tadashi	The Society of Rheology, Japan, Research Award
	KAWACHI, Atsushi	The Society of Silicon Chemistry, Japan Award for Young Chemists
	SUGIURA, Yukio	The Pharmaceutical Society of Japan Award
2001	MURAKAMI, Syozo	The Chemical Society of Japan Award for Technical Achievements
	MATUBAYASI, Nobuyuki	Helmholtz Award, International Association for the Properties of Water and Steam
	UCHINO, Takashi	Vittorio Gottardi Prize, International Commission on Glass
	TAKAHASHI, Masahide	The Ceramic Society of Japan, Young Scientists Award
	OSAKI, Kunihiro	The Society of Rheology, Japan, Award
	KAWACHI, Atsushi	The Chemical Society of Japan Award for Distinguished Young Chemists
2002	AZUMA, Masaki	Japan Sociey of Powder and Powder Metallurgy Award for Innovatory Research
	KANAYA, Toshiji	The Society of Fiber Science and Technology, Japan Prize for Excellence in Fiber Reserch
	KOMATSU, Koichi	Alexander von Humboldt Research Award
	TAMAO, Kohei	The 42nd Toray Science & Technology Prize (2002) (Toray Science Foundation)
	TAMAO, Kohei	Frederic Stanley Kipping Award 2002, The American Chemical Society
	YAMAGUCHI, Shigehiro	The Chemical Society of Japan Award for Distinguished Young Chemists
2003	KURATA, Hiroki	The Japanese Society of Microscopy Award (Setou Award)
	SOHRIN, Yoshiki	18th Oceanochemistry Award (Research Institute of Oceanochemistry)
	TAKAHASHI, Masahide	Ceramic Society of Japan/The Australasian Ceramic Society (CJS/ACS) Joint Ceramic Award for 2003
	TOKITOH, Norihiro	The Division Award of The Chemical Society of Japan
	TAMAO, Kohei	The Asahi Prize 2002 (Asahi Culture Foundation)
	TAMAO, Kohei	The 14th Mukai Prize (Tokyo Ohka Foundation for the Promotion of Science and Technology)
	TAKANO, Mikio	2002 JSPM Award for Distinguished Achievements in Research

Educational and Social Activities

Theses

	Science	Engineering	Agricultural Sc	Medical Sc	Pharmaceutial Sc	Total
2001	13	17	1	1	2	34
2002	15	9	2	5	0	31

Lectures

(April 1, 2002 - March 31, 2003)

2002	June 22	9th Public Lectures "Advanced Manufacturing Technologies: Challenge of the Institute for Chemical Research"
	August 23	5th Chemistry for High School Students - Lectures and Open Laboratories "Hear, See and Enjoy the Frontiers of Chemistry"
	September 28	6th Open Campus Uji 2002 (collaboration)
	December 6	102nd Annual Symposium of Institute for Chemical Research
2003	February 21	Symposium of Graduate Students

Publications

(April 1, 2002 - March 31, 2003)

ICR Annual Report 2002, vol. 9
Profiles of Institute for Chemical Research 2002 (in Japanese)
Obaku (News Letter of Institute for Chemical Research, in Japanese), No. 17, 18

Web Pages

http://www.kuicr.kyoto-u.ac.jp/index_J.html
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Desk for Administration Department／NAGASAKI, Junichi　MIYAMOTO, Mariko
KOBAYASHI, Sayuri　NISHIMURA, Maki
Public Relations Section／UENOYAMA, Mika　KARIKOMI, Miwako

Successive Directors

1	CHIKASHIGE, Masumi	1927～1930	16	SHIGEMATSU, Tsunenobu	1976～1978
2	KITA, Gen-itsu	1930～1942	17	TASHIRO, Megumi	1978～1980
3	HORIBA, Shinkichi	1942～1945	18	TAKADA, Toshio	1980～1982
4	KONDO, Kinsuke	1945～1946	19	FUJITA, Eiichi	1982～1984
5	NOZU, Ryuzaburo	1946～1948	20	INAGAKI, Hiroshi	1984～1986
6	UCHINO, Senji	1948～1953	21	KURATA, Michio	1986～1988
7	HORIO, Masao	1953～1956	22	TAKANAMI, Mituru	1988～1990
8	TAKEI, Sankichi	1956～1959	23	SAKKA, Sumio	1990～1992
9	NAKAI, Risaburo	1959～1961	24	ODA, Jun-ichi	1992～1994
10	GOTO, Renpei	1961～1964	25	MIYAMOTO, Takeaki	1994～1996
11	KUNICHIKA, Sango	1964～1967	26	SHINJO, Teruya	1996～1998
12	TSUJI, Waichiro	1967～1970	27	SUGIURA, Yukio	1998～2000
13	KUNICHIKA, Sango	1970～1972	28	TAMAO, Kohei	2000～2002
14	SUITO, Eiji	1972～1974	29	TAKANO, Mikio	2002～2004
15	TAKEZAKI, Yoshimasa	1974～1976			

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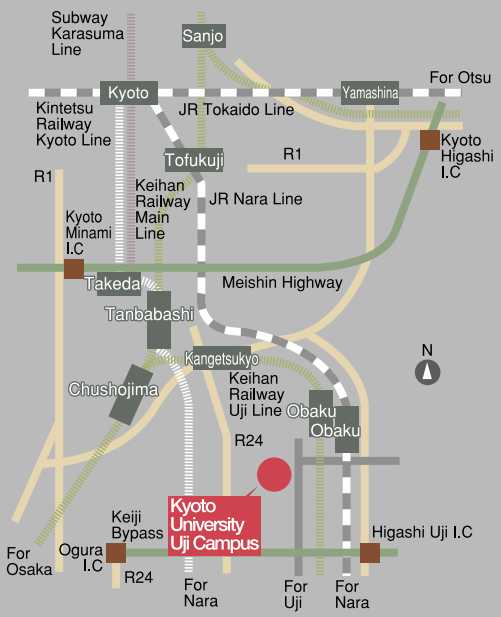

Location and Transportation

From Obaku Station on the Keihan Uji Line: 10 min by walk
(from Keihan-Sanjo Station to Obaku Station: 35 min)
From Obaku Station on the JR Nara Line: 7 min by walk
(from Kyoto Station to Obaku Station: 20 min)
From Kyoto-Minami Interchange: 20 min by car
From Uji-Higashi Interchange: 10 min by car