

I N S T I T U T E

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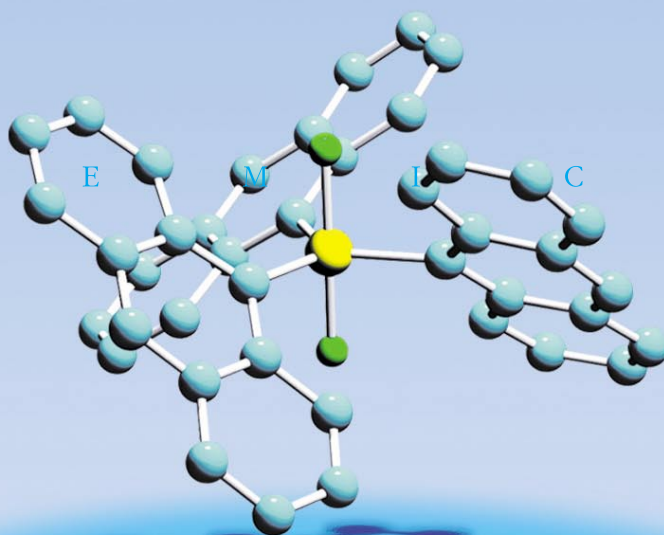
C H E M I C A L

R E S E A R C H

K Y O T O

The Institute For Chemical Research
Kyoto University
2002

U N I V E R S I T Y





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Director
TAKANO, Mikio

The Institute for Chemical Research of Kyoto University celebrated its 75th anniversary in 2001, the first year of the 21st century. The institute 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-attached research institute in Japan. For 75 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 our noble doctrine, "Conducting Fundamental Studies and Exploring Their Application to Special Fields of Chemistry".

The research activities of the Institute encompass organic chemistry, inorganic chemistry, biochemistry, materials chemistry and physical chemistry. The organization of the Institute was changed from the laboratory system to the division system in 1992, and more recently the Bioinformatics Center was established in 2001. The present system includes nine divisions and two affiliated research centers, which at the present time consists of a total of 29 laboratories and three guest-laboratories. Currently, each laboratory is affiliated with one of the Graduate Schools: Science, Engineering, Agriculture, Pharmaceutical Sciences, Medicine, or Informatics.

The Bioinformatics Center, which introduced a new massively parallel super computer system in January of 2002, plays an active role as one of the main bioinformatics centers in Japan and the world. In April of this year, the Laboratory of Proteome Informatics (donated by SGI Japan) started its activity to develop novel computational techniques to elucidate systematic principles of protein interactions. Thus, the center promotes new research activities in order to understand how life operates by analyzing complex interactions among building blocks and dynamic environments. The center will also contribute to the economy and the social welfare by developing

novel bioinformatics technologies to utilize the genome and proteome information.

The Kyoto University Center of Excellence (COE) Project entitled "Elements Science" started in 2000 and heralded the first center in the field of engineering and science at Kyoto University. Our Institute plays a key role in this newly organized effort.

In 2001, a new research network involving physics and chemistry was started based on collaborations between five large institutes in Japan including our institute.

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

June, 2002

Mikio Takano

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 Gokasyo, 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 satellite 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 ICR started a new research program "Collaboratory on Electron Correlations - Towards a New Research Network between Physics and Chemistry"
Bioinformatics Center was established

Divisions and Their Historical Backgrounds

Original Research Subject	Primary Stage	Secondary Stage	Present Division	Graduate School
1939 Nuclear Physics	Nuclear Reaction 1964 Nuclear Science R.F.	Nuclear Science R.F.	Nuclear Science R.F.	S
1941 Reaction in Gas Explosion	Crystal and Powder Chemistry 1956 Nuclear Radiation 1956 Polymer Crystals		States and Structures	S·E
1933 Colloidal Drugs·Paints 1944 Dielectrics	Surface Chemistry Dielectrics 1956 Radiochemistry		Interface Science	S
1929 Alloys 1939 Special Glass	Solid State Chemistry Ceramic Chemistry	Solid State Chemistry	Solid State Chemistry	S·E
1939 Rubbers, Resins and Plastics 1943 Synthetic Fibers	Polymer Physical Chemistry Fiber Chemistry	Fundamental Material Properties	Fundamental Material Properties	E
1937 Synthetic Wool 1937 Liquid Fuels	Polymer Separation and Characterization High Pressure Chemistry		Organic Materials Chemistry	E
	1958 Petroleum Chemistry		Synthetic Organic Chemistry	E·P
1926 Production of Saviol	Physiological Activity	Cancer Drug Research		
1943 Organic Resources	Organic Unit Reaction		Bioorganic Chemistry	S·P·M
1944 Pyrethroids·Mint Oils 1933 Exploitation of Tundra	Plant Products Chemistry Microbial Biochemistry		Biofunctional Molecules	A
1929 Chemistry of Nutrition 1929 Bacteria and Fungi 1944 Fermentation	Physical Chemistry of Enzyme Molecular Biology	1985 Molecular Design for Physiological Functions	Molecular Biology and Information Science	S
		1981 Nucleic Acids Lab.		
			2001 Bioinformatics Center	S·I
			(1992.4.)	
			2002 Contributed Chair Proteome Informatics (SGI Japan)	

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

(As of May 1 2002)

Research Division	Subdivision (Laboratory)	Professor	Associate Professor	Instructor	Technician
States and Structure	I. Atomic and Molecular Physics	— HATA, Yasuo	— ITO, Yoshiaki	— NAKAMATSU, Hirohide	
	II. Electron Microscopy and Crystal Chemistry	— ISODA, Seiji	— KURATA, Hiroki	— OGAWA, Tetsuya — NEMOTO, Takashi	— MORIGUCHI, Sakumi
	III. Polymer Condensed States	— KOHJIYA, Shinzo	— TSUJI, Masaki	— URAYAMA, Kenji — TOSAKA, Masatoshi	
Interface Science	I. Solutions and Interfaces	— NAKAHARA, Masaru	— UMEMURA, Junzo	— MATSUMOTO, Mutsuo — MATUBAYASI, Nobuyuki — OKAMURA, Emiko	— WAKAI, Chihiro
	II. Molecular Aggregates	— SATO, Naoki	— ASAMI, Koji	— KITA, Yasuo — YOSHIDA, Hiroyuki	
	III. Hydrospheric Environment Analysis	— SOHRIN, Yoshiki	— UMETANI, Shigeo	— SASAKI, Yoshihiro — OKAMURA, Kei	— NORISUYE, Kazuhiro — MINAMI, Tomoharu
Solid State Chemistry	I. Artificial Lattice Alloys	— (Vacancy)	— (Vacancy)	— FUJITA, Masaki	
	II. Quantum Spin Fluids	— YAMADA, Kazuyoshi	— (Vacancy)	— IKEDA, Yasunori	
	III. Solid State Chemistry	— TAKANO, Mikio	— TERASHIMA, Takahito	— AZUMA, Masaki	
	IV. Amorphous Materials	— YOKO, Toshinobu	— (Vacancy)	— TAKAHASHI, Masahide — SHIMADA, Ryoko	
	G. Structure Analysis	— KANNO, Ryoji	— MITANI, Seiji		
Fundamental Material Properties	I. Molecular Rheology	— (Vacancy)	— WATANABE, Hiroshi	— INOUE, Tadashi	— OKADA, Shinichi
	II. Polymer Materials Science	— (Vacancy)	— KANAYA, Toshiji	— NISHIDA, Koji	
	III. Molecular Dynamic Characteristics	— HORII, Fumitaka	— TSUNASHIMA, Yoshisuke	— KAJI, Hironori — HIRAI, Asako	— OHMINE, Kyoko
	G. Composite Material Properties	— YAMAMOTO, Yasushi	— SAITO, Hiromu		
Organic Materials Chemistry	I. Polymeric Materials	— FUKUDA, Takeshi	— TSUJII, Yoshinobu	— MURAKAMI, Syozo — OHNO, Kohji — GOTO, Atsushi	
	II. Organic Structural Chemistry	— KOMATSU, Koichi	— KITAGAWA, Toshikazu	— NISHINAGA, Tohru — MURATA, Yasujiro	
Synthetic Organic Chemistry	I. Synthetic Design	— TAMAO, Kohei	— (Vacancy)	— YAMAGUCHI, Shigehiro — TSUJI, Hayoto	
	II. Fine Organic Synthesis	— (Vacancy)	— KAWABATA, Takeo	— TSUBAKI, Kazunori	— TERADA, Tomoko
	G. Synthetic Theory	— NAKA, Takehiko	— SUGIHARA, Takumichi		
Bioorganic Chemistry	I. Organoelement Chemistry	— TOKITOH, Norihiro	— NAKAMURA, Kaoru	— SUGIYAMA, Takashi — KAWAI, Yasushi — TAKEDA, Nobuhiro	— YAMAZAKI, Norimasa — HIRANO, Toshiko
	II. Bioactive Chemistry	— SUGIURA, Yukio	— FUTAKI, Shiroh	— NAGAOKA, Makoto	
	III. Molecular Clinical Chemistry	— UEDA, Kunihiko	— TANAKA, Seigo		
Molecular Biofunction	I. Chemistry of Molecular Biocatalysts	— SAKATA, Kanzo	— HIRATAKE, Jun	— MIZUTANI, Masaharu — SHIMIZU, Bun-ichi	
	II. Molecular Microbial Science	— ESAKI, Nobuyoshi	— YOSHIMURA, Tohru	— KURIHARA, Tatsuo — MIHARA, Hisaaki	
Molecular Biology and Information	I. Biopolymer Structure	— (Vacancy)	— (Vacancy)	— HIRAGI, Yuzuru — FUJII, Tomomi	
	II. Molecular Biology	— OKA, Atsuhiko	— AOYAMA, Takashi	— SAKAI, Hiroe — KAWASHIMA, Shuichi	— YASUDA, Keiko
Bioinformatics Center	I. Bioknowledge Systems	— KANEHISA, Minoru	— GOTO, Susumu	— NAKAYA, Akihiro	
	II. Biological Information Network	— AKUTSU, Tatsuya [Adjunct prof]	— SUGISAKI, Hiroyuki	— UEDA, Nobuhisa	
	III. Pathway Engineering	— MIYANO, Satoru [Section head]	— (Vacancy)		
Supercomputer Laboratory	— KANEHISA, Minoru				
Contributed Chair	— Proteome Informatics (SGI Japan)		— MAMITSUKA, Hiroshi	— YAMAGUCHI, Atsuko	
Nuclear Science Research Facility	I. Particle and Photon Beams	— NODA, Akira	— IWASHITA, Yoshihisa	— SHIRAI, Toshiyuki	— TONGUU, Hiromu
	II. Beams and Fundamental Reaction	— (Vacancy)	— MATSUKI, Seishi		
Low Temperature Laboratory					— KUSUDA, Toshiyuki
Centoral Work-Shop					— IMANISHI, Katsumi — KAZAMA, Ichiro

(G : Laboratory for Visiting Professor)

Atomic and Molecular Physics

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Prof. HATA, Yasuo (D Sc)
Assoc. Prof. ITO, Yoshiaki (D Sc)
Instructor NAKAMATSU, Hirohide (D Sc)

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.

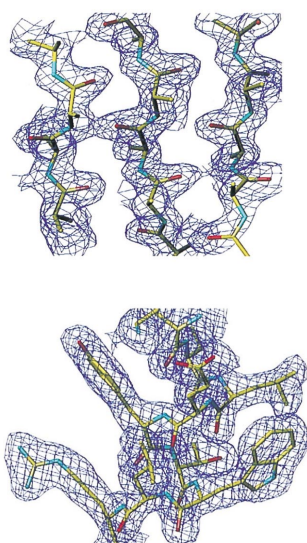


Figure legend: Electron density map of a protein molecule

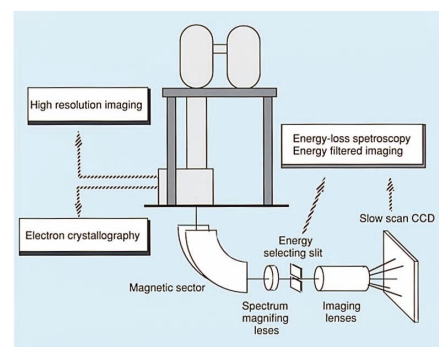
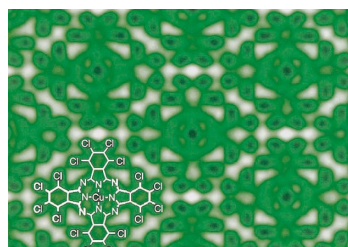
Electron Microscopy and Crystal Chemistry

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Prof. ISODA, Seiji (D Sc)
Assoc. Prof. KURATA, Hiroki (D Sc)
Instructor OGAWA, Tetsuya (D Sc)
NEMOTO, Takashi (D Sc)
Assoc. Instr. MORIGUCHI, Sakumi

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.



Polymer Condensed States

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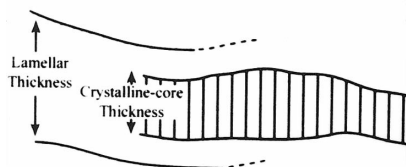
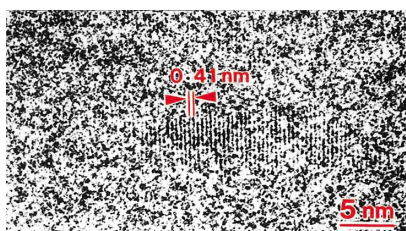
Prof. KOHJIYA, Shinzo (D Eng)

Assoc. Prof. TSUJI, Masaki (D Eng)

Instructor URAYAMA, Kenji (D Eng)

TOSAKA, Masatoshi (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-oxotriethylene) 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.

Solutions and Interfaces

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Prof. NAKAHARA, Masaru (D Sc)

Assoc. Prof. UMEMURA, Junzo (D Sc)

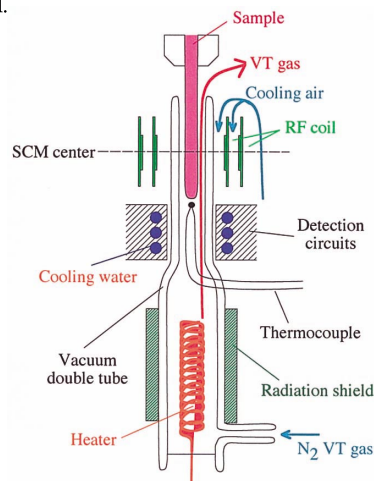
Instructor MATSUMOTO, Mutsuo (D Sc)

MATUBAYASI, Nobuyuki (Ph D)

OKAMURA, Emiko (D Pharm Sc)

Assoc. Instr. 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 super-cooled. 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

Molecular Aggregates

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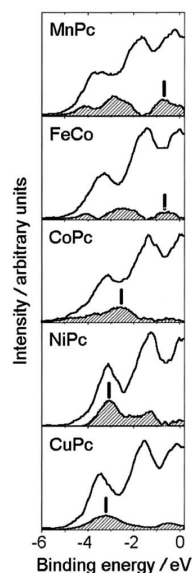
Prof. SATO, Naoki (D Sc)
Assoc. Prof. ASAMI, Koji (D Sc)
Instructor KITA, Yasuo (D Sc)
YOSHIDA, Hiroyuki (D Sc)

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 methylation 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.



Hydrospheric Environment Analysis

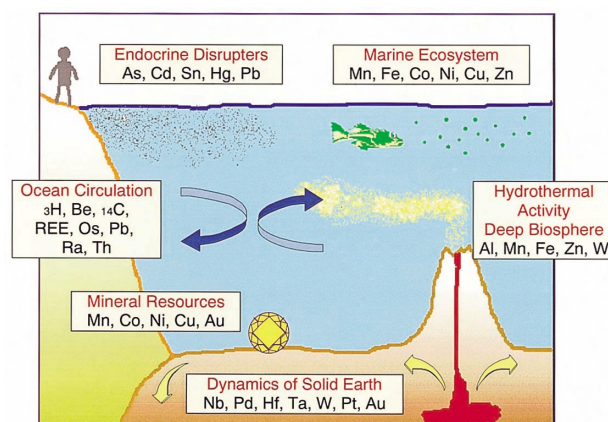
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Prof. SOHRIN, Yoshiki (D Sc)
Assoc. Prof. UMETANI, Shigeo (D Sc)
Instructor SASAKI, Yoshihiro (D Sc)
OKAMURA, Kei (D Sc)
Assoc. Instr. NORISUYE, Kazuhiro
MINAMI, Tomoharu

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 CO₂ 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.



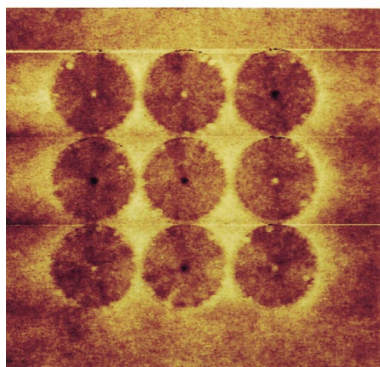
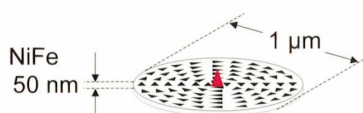
Artificial Lattice Alloys

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Prof. SHINJO, Teruya
retired on March, 2002

Instructor FUJITA, Masaki (D Sc)
Technician KUSUDA, Toshiyuki

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.



Quantum Spin Fluids

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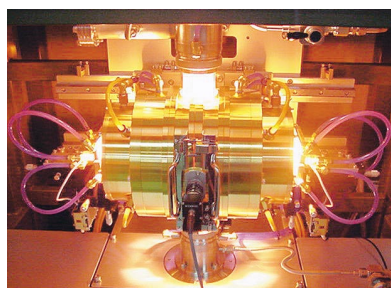


Prof. YAMADA, Kazuyoshi (D Sc)
Instructor IKEDA, Yasunori

Discovery of the high- T_c superconductor of cuprates and study on its mechanism stimulated many other researches relating with the interplay between magnetism and electric transport properties. Nowadays these researches formed one of the main fields in the condensed matter science.

Intensive studies in this field, which is called the strongly correlated electron system (SCES), have revealed that the competition and/or coexistence between distinct phases or the microscopic phase separation is observed in many cases. Inhomogeneous electron distribution in SCES is expected to show some quantum properties due to its dynamical nature. Novel properties in SCES such as high- T_c Superconductivity are considered to take place in the above situation.

In order to elucidate the novel properties in SCES we have been performing experimental research on the interplay between microscopic magnetism and electrical phenomena such as superconductivity and metal-insulator transitions. Explicitly, we systematically grow large and impurity-free single crystals mainly for transition metal oxides and sulfides and investigate the physical properties. With single crystals such as $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ spin and lattice dynamics are investigated by inelastic neutron scattering. Recently, we have started inelastic x-ray scattering measurements utilizing synchrotron x-ray in order to directly observe the charge fluctuations in superconducting state.



Double ellipsoidal infra-red image furnace for growth of single crystal

Solid State Chemistry

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Prof. TAKANO, Mikio (D Sc)
Assoc. Prof. TERASHIMA, Takahito (D Sc)
Instructor AZUMA, Masaki (D Sc)

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 (5GPa and 1000°C, typically), film growth (pulsed laser ablation), and microscopic fabrication.

In the focus of our interest are manganese oxides showing colossal magnetoresistance, Fe⁴⁺-oxides like SrFeO₃ showing properties dominated by oxygen p-hole character, Ni³⁺-oxides like BiNiO₃ showing quantum mechanical properties involving the charge, spin, and orbital degrees of freedom, cupric oxides suitable for experiments to clarify the mechanism of high-Tc superconductivity like (Ca,Na)₂CuO₂Cl₂, SrCu₂O₃ (two-legged ladder), and Sr₂Cu₃O₅ (three-legged ladder).

The most remarkable technical progress about the high-pressure synthesis is of single crystal growth. Shown in the figure are the crystals of CaFeO₃ (a), (Ca,Na)₂CuO₂Cl₂ (b), (VO)₂P₂O₇ (c) and Tl₂Ru₂O₇ (d) grown at 3 to 4.5 GPa and 1300 °C Concerning films, we have succeeded in establishing the techniques needed to study the FET effects.

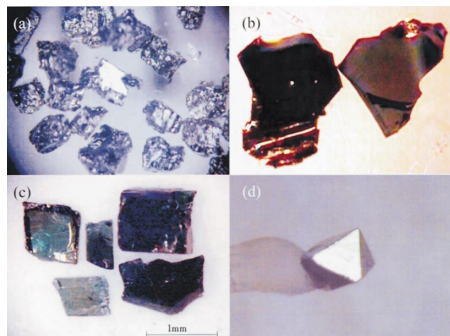


Fig : Single crystals of CaFeO₃ (a), (Ca,Na)₂CuO₂Cl₂ (b), (VO)₂P₂O₇ (c) and Tl₂Ru₂O₇ (d) grown at 3 to 4.5 GPa and 1300°C.

Amorphous Materials

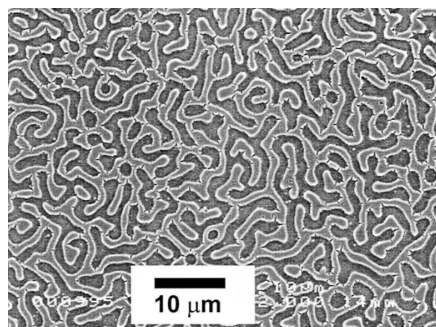
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Prof. YOKO, Toshinobu (D Eng)
Instructor TAKAHASHI, Masahide (D Sc)
SHIMADA, Ryoko (D Sc)

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.



TiO₂ Thin film with two-dimensional spinodal-phase separation structure prepared by the sol-gel method

Molecular Rheology

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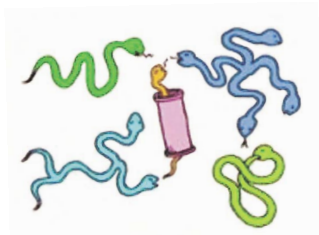
Prof. OSAKI, Kunihiro
retired on March, 2002

Assoc. Prof. WATANABE, Hiroshi (D Sc)
Instructor INOUE, Tadashi (D Eng)
Technician OKADA, Shinichi

Rheology is a research area to investigate the relationship of stress and strain of materials. Polymeric materials are viscoelastic, i. e., the modulus varies with frequency of deformation. They can be glassy, rubbery, or liquid-like, depending on chemical structure, temperature, and frequency. This variety of rheological features gives rise to the excellent material properties and good processability.

Our aim is to clarify the microscopic origin of rheological behavior, which is related to molecular motions in materials of various structures: polymer melts, polymer solutions, glassy polymers, block copolymers with micro-domain structures, liquid crystalline polymers, dispersion of solid particles in polymeric material, and surfactant micelles. Anionic polymerization is utilized to produce model branched polymers and block copolymers. The molecular motion related to rheology is sought through combined measurements of stress (rheometry), dielectric relaxation, and birefringence of deformed materials. Infrared dichroism measurement is also used for multi-component systems and liquid crystals. Cooperative applied studies are also in progress.

- (1) Improvement of polymer processing technology.
- (2) Molecular design of polyolefins for various products.
- (3) Development of low-birefringent polymers.
- (4) New polymeric gels.
- (5) Development of substitute for polyvinyl chloride.
- (6) Stability of paint.



Motion of entangled polymer chain is similar to the motion of a snake in an earthen pipe. Motion of a branched snake in a branched tube is one of the present subjects of this group.

Polymer Materials Science

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Instructor NISHIDA, Koji (D Eng)

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) We found a surprising phenomenon that during the induction period of polymer crystallization a spinodal decomposition type microphase separation due to orientational fluctuations occurs (see the Photo). (2) Freezing 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.

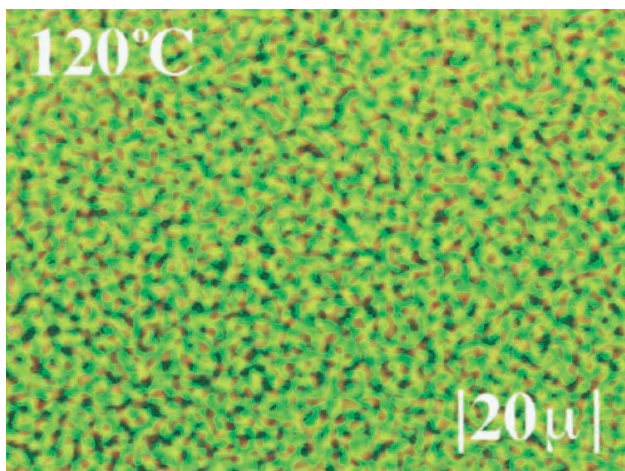


Photo: Light micrograph of PET showing a spinodal decomposition type microphase separation at very initial stage of crystallization. Bright parts indicate the domains where the parallel orientation of chain segments is advanced and crystallization initiates first.

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.

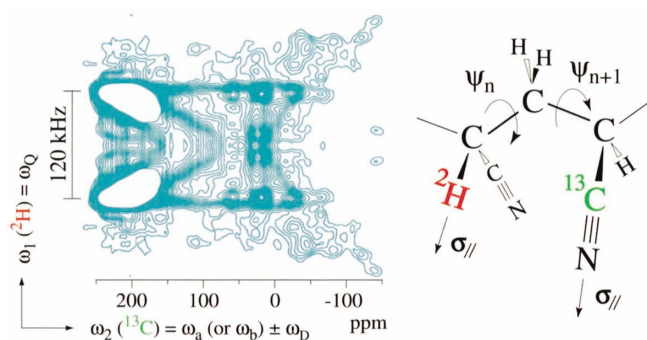
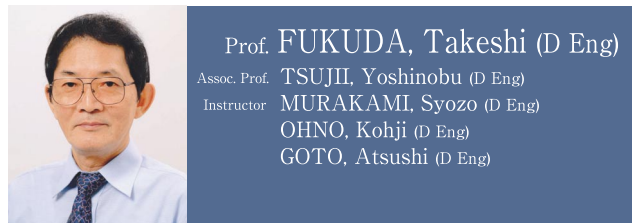


Figure
Precise analysis of the conformation of solid polyacrylonitrile by 2D solid-state heteronuclear multiple quantum coherence NMR.

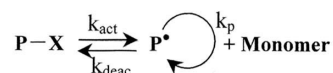
Polymeric Materials

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Kinetic and mechanistic analyses are made for better understandings and systematization of the chemical and physico-chemical 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).

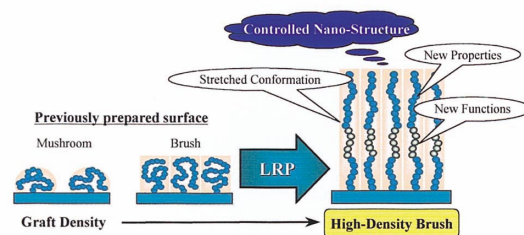


• Nitroxide-mediated polymerization (NMP), Atom transfer radical polymerization (ATRP), Reversible addition-fragmentation chain transfer (RAFT) polymerization

(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

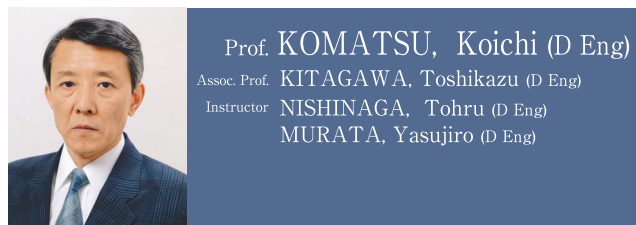
(3) Synthesis, properties, and applications of high-density polymer brushes.



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

Organic Structural Chemistry

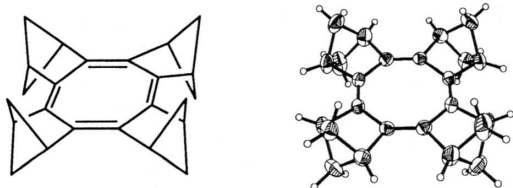
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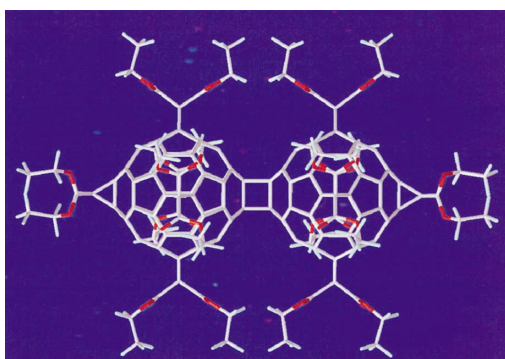
Synthetic, structural, and theoretical studies are being conducted on π -conjugated hydrocarbon molecules, with particular attention being paid for the redox activity. Thus, structural features are pursued to create stable cationic and radical species in order to furnish redox-active systems as fundamental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



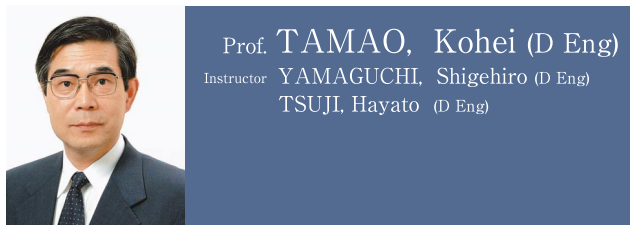
The first planarized and amphoteric cyclooctatetraene.



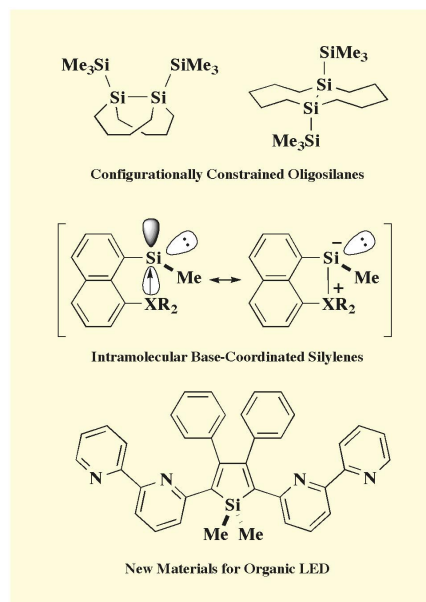
Symmetrically functionalized fullerene dimer, $C_{130}(CO_2Et)_{20}$.

Synthetic Design

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Our research interests encompass elements science, molecular science, and materials science. Current research projects are concerned with the development and application of new synthetic methodologies and new functions of organic compounds of the main group elements, focusing on silicon, boron and some others. They include (1) π -conjugated systems containing silole, borole, and trianthryl-element moieties, for application to electroluminescent devices etc., (2) penta-coordinated silicon compounds, aiming at new functions, (3) functionalized silyl anions, as new synthetic reagents, (4) divalent silicon species aiming at new functions, and (5) oligosilanes and polysilanes for full understanding of the sigma-conjugation. Some examples are shown below.



Fine Organic Synthesis

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Prof. FUJII, Kaoru retired on March, 2002	Assoc. Prof. KAWABATA, Takeo (D Pharm. Sc) Instructor TSUBAKI, Kazunori (D Pharm. Sc) Technician TERADA, Tomoko
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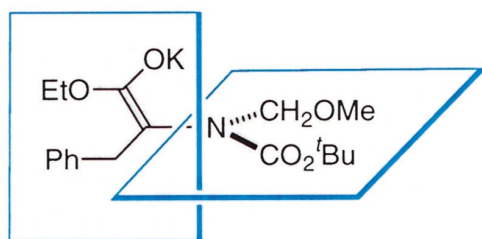
Research in this laboratory focuses on chirality, especially on the development of new methods for asymmetric synthesis and chiral molecular recognition.

(I) Asymmetric Synthesis

Studies include (1) asymmetric synthesis of quaternary carbon centers through addition-elimination process, (2) asymmetric induction based on a new concept "memory of chirality", (3) use of optically active binaphthyls for asymmetric synthesis, (4) kinetic resolution by chiral nucleophilic catalysts, and (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 hexahomooxalix[3]arenes are employed for the capture of guest molecules. Phenolphthalein and spiropyranes are used as chromophore. Optically active binaphthyls 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.

Organoelement Chemistry

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Prof. TOKITOH, Norihiro (D Sc)
Assoc. Prof. NAKAMURA, Kaoru (D Sc)
Instructor SUGIYAMA, Takashi (D Sc)
KAWAI, Yasushi (D Sc)
TAKEDA, Nobuhiro (D Sc)
Assoc. Instr. YAMAZAKI, Norimasa (D Sc)
Technician HIRANO, Toshiko

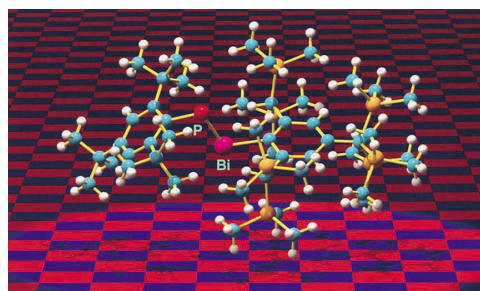
Organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of "dreams" for organic chemists. In recent years, however, remarkable 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 metallaromatic compounds containing a silicon or germanium atom" and "the first stable doubly bonded system between the third and sixth row main group elements (phospha-bismuthene)" 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

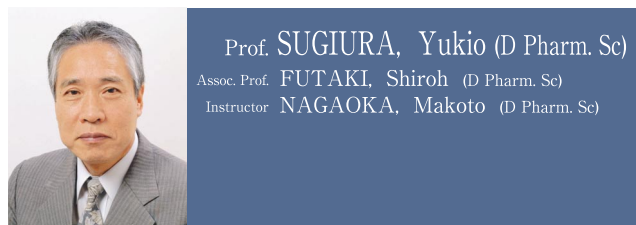
New synthetic applications mediated by biocatalysts (microorganisms, cells of plants, and enzymes) are studied. Further extension of biocatalysts to the detoxication of environmental pollution substances is also under way.



Molecular Structure of a Kinetically Stabilized P=Bi Double-bond Compound (Phospha-bismuthene)

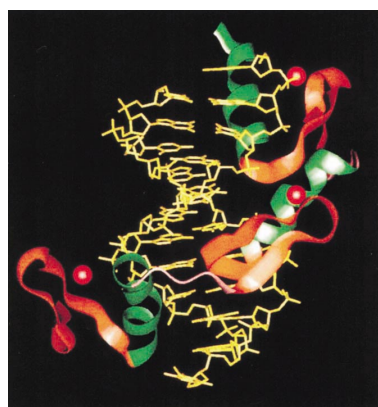
Bioactive Chemistry

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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

Molecular Clinical Chemistry

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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.

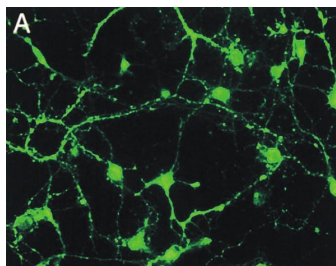


Fig.1. Primary culture of rat neuronal cells (immunostaining with anti-neurofilament antibody, x400)

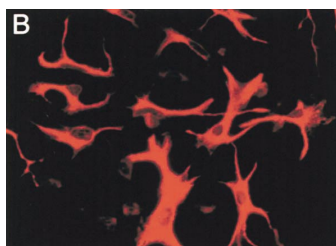


Fig.2. Primary culture of rat glial cells (immunostaining with anti-GFAP antibody, x400)

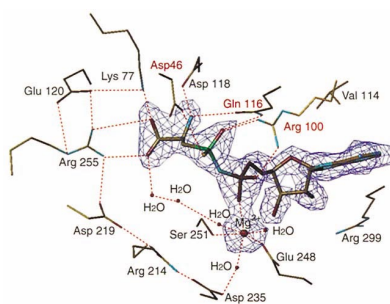
Chemistry of Molecular Biocatalysts

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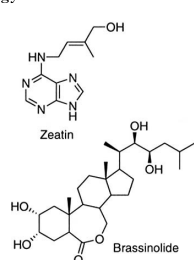
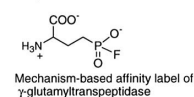
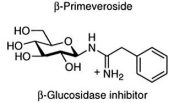
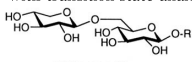


Prof. SAKATA, Kanzo (D Agr)
Assoc. Prof. HIRATAKE, Jun (D Agr)
Instructor MIZUTANI, Masaharu (D Agr)
SHIMIZU, Bun-ichi (D Agr)

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



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



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.

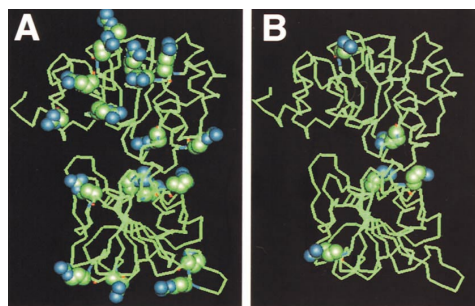
Molecular Microbial Science

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Assoc. Prof. YOSHIMURA, Tohru (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.

Biopolymer Structure

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Instructor HIRAGI, Yuzuru (D Sc)
FUJII, Tomomi (D Sc)

Protein is an important constituent of the living organism and functions when it adopts its own stereostructure directed by its amino acid sequence; in short, the structure of protein defines its function. This laboratory aims at elucidating the structure-function relationships of protein and the principles of protein architecture based on its crystal and/or solution structures determined by X-ray analyses. The main research themes are as follows; (1) structure determination of biologically important proteins by X-ray crystallography, and crystallographic studies on functional mechanisms of the proteins, such as enzymatic reaction and protein thermostabilization, (2) small-angle X-ray-solution-scattering studies on assembly of oligomeric proteins, and (3) physicochemical studies on assembly of myosin molecules into thick filaments. Recent results of theme (1) are crystallographic elucidations of the reaction mechanisms of the *Pseudomonas aeruginosa* alkaline protease, the L-2-haloacid dehalogenase, the NifS-homologous enzyme and the thermostable aspartase, and of the thermostabilization mechanisms of the oligo-1,6-glucosidase and the archaeal ferredoxin; those of theme (2) are biophysical clarifications of the mechanisms of multicomponent assembly in tobacco mosaic virus and chaperonin GroEL; those of theme (3) are physicochemical elucidations of the axial-stagger mechanism of skeletal muscle myosin.



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

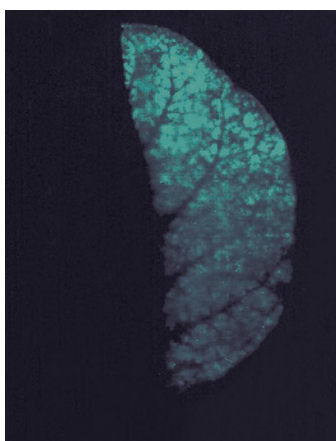
Molecular Biology

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Assoc. Prof. AOYAMA, Takashi (D Sc)
Instructor SAKAI, Hiroe (D Sc)
KAWASHIMA, Shuichi
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.

Bioknowledge Systems

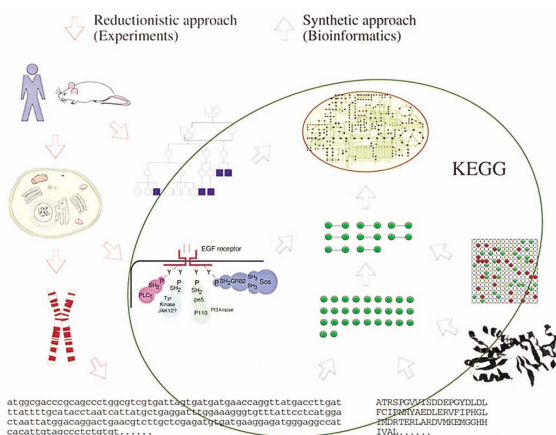
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Prof. KANEHISA, Minoru (D Sc)
 Assoc. Prof. GOTO, Susumu (D Eng)
 Instructor NAKAYA, Akihiro (D Sc)

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/>).



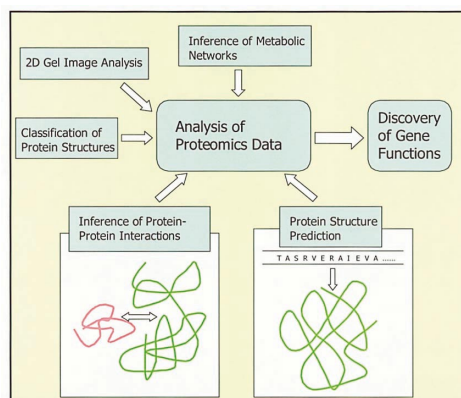
Biological Information Network

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Prof. AKUTSU, Tatsuya (D Eng)
 Assoc. Prof. SUGISAKI, Hiroyuki (D Sc)
 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.



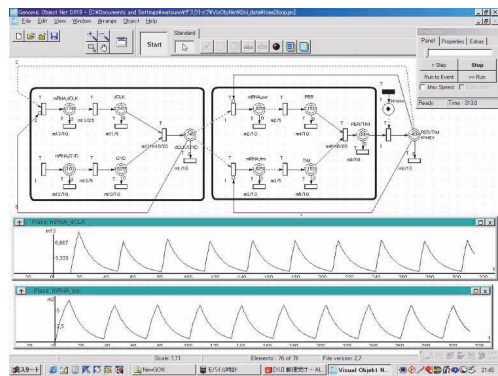
Pathway Engineering

Tel : 0774-38-3293 Fax : Pending
e-mail : miyanolab@kuicr.kyoto-u.ac.jp



Prof. MIYANO, Satoru (D Sc)
[Adjunct professor]

This laboratory develops research on computational knowledge discovery, e.g. inference of pathway information from gene expression profile data, and simulation system for cells and organisms through the biopathway simulation of gene regulatory networks, signaling pathways, metabolic pathways, and physical simulations, etc. With this approach, the functions of genes and systems of genes will be analyzed and predicted. These researches are realized as a software library HypothesisCreator (<http://www.HypothesisCreator.Net/>) and a biopathway simulation system Genomic Object Net (<http://www.GenomicObject.Net/>).



Snapshot of Genomic Object Net: Simulation of circadian rhythm

Particle and Photon Beams

Tel : 0774-38-3281 Fax : 0774-38-3289
e-mail : (user name)@kyticr.kuicr.kyoto-u.ac.jp



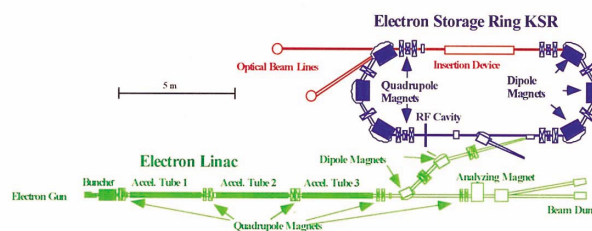
Prof. NODA, Akira (D Sc)
Assoc. Prof. IWASHITA, Yoshihisa (D Sc)
Instructor SHIRAI, Toshiyuki
Technician TONGUU, Hiromu

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 proton 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 proton synchrotron has been developed.



Layout of the Electron Accelerator

Beams and Fundamental Reaction

Tel : 0774-38-3292 Fax : 0774-38-3289
e-mail : (user name)@carrack.kuicr.kyoto-u.ac.jp

Assoc. Prof. MATSUKI, Seishi (D Sc)

Atoms, nuclei and particles are studied with the quantum electronic method.

1) Properties of highly excited Rydberg states in alkali atoms with the principal quantum number n ranging from 50 to 150, are investigated with the selective field ionization detection, following the multi-step laser excitations of them. Subjects being studied are Stark polarizabilities, avoided crossings, adiabatic and non-adiabatic transitions in ramped electric field, and the coherent time evolution in a pulsed electric field. Also applications of Rydberg atoms to fundamental physics research, especially to cavity QED and to ultra low-noise microwave single-photon detector are developed.

2) Nuclear magnetism in 3-5 semiconductor materials are studied with laser optical pumping and pulsed nuclear magnetic resonance. Especially interested substance is the semiconductor InP, in which nuclei are polarized with lasers in self-polarization mode. Due to the strong hyperfine coupling between the nuclei and the electrons in the conduction band, the nuclei can be completely polarized below some critical temperature, occurring a kind of ferromagnetic phase transition. This phase transition observed for the first time in InP by us is being studied in detail.

3) Axions, invoked to solve the so-called strong CP problem in QCD theory, are one of the leading candidates for the cold dark matter particles in the Universe.

Axions with its mass from 2 to 30 micro-electron-volts are searched with the Rydberg-atom cavity detector: In this scheme, axions are converted into microwave photons in a strong magnetic field (about 7 T) and the axion-converted photons are absorbed by highly excited Rydberg atoms and the excited atoms are then selectively detected by the field



ionization method. Following the prototype apparatus called CARRACK1, a large-scale dark matter axion search apparatus CARRACK2 was constructed and the search over a wide range of axion mass is in progress with this new system.

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
[Instructor] YAMAGUCHI, Atsuko

Sequencing has been completed for genomes of more than fifty different organisms.

Even the completion of sequencing human genome is now almost at hand. The focus has shifted from simple genome sequencing to deep understanding of complicated interactive relations of proteins (gene products).

A set of protein relations, such as protein-protein and protein-ligand interactions etc., is called a proteome. "Proteome informatics" is a new research field to analyze the proteomes with information processing techniques. The objectives of this laboratory are to promote the researches in proteome informatics and to develop novel computational techniques to elucidate systematic principles of the proteomes.

Nobel Prize

(period of one's tenure of ICR)

YUKAWA, Hideki	1949	Physics	(1943~1968)
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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

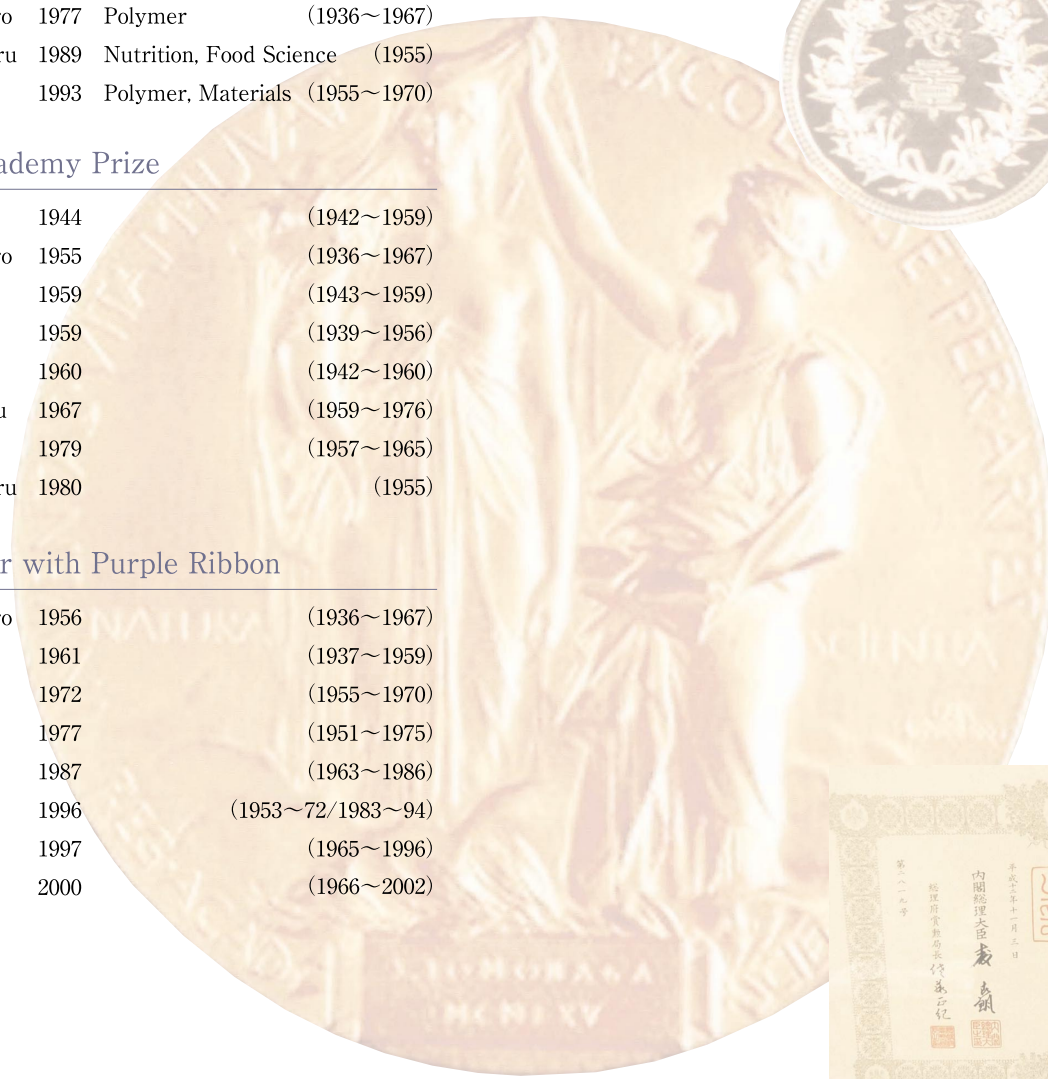
YUKAWA, Hideki	1951	Atomic Physics	(1943~1968)
HORIBA, Shinkichi	1966	Physical Chemistry	(1927~1947)
HAYAISHI, Osamu	1972	Biochemistry	(1959~1976)
SAKURADA, Ichiro	1977	Polymer	(1936~1967)
MITSUDA, Hisateru	1989	Nutrition, Food Science	(1955)
HORIO, Masao	1993	Polymer, Materials	(1955~1970)

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)
TAKEL, 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



① Main Building



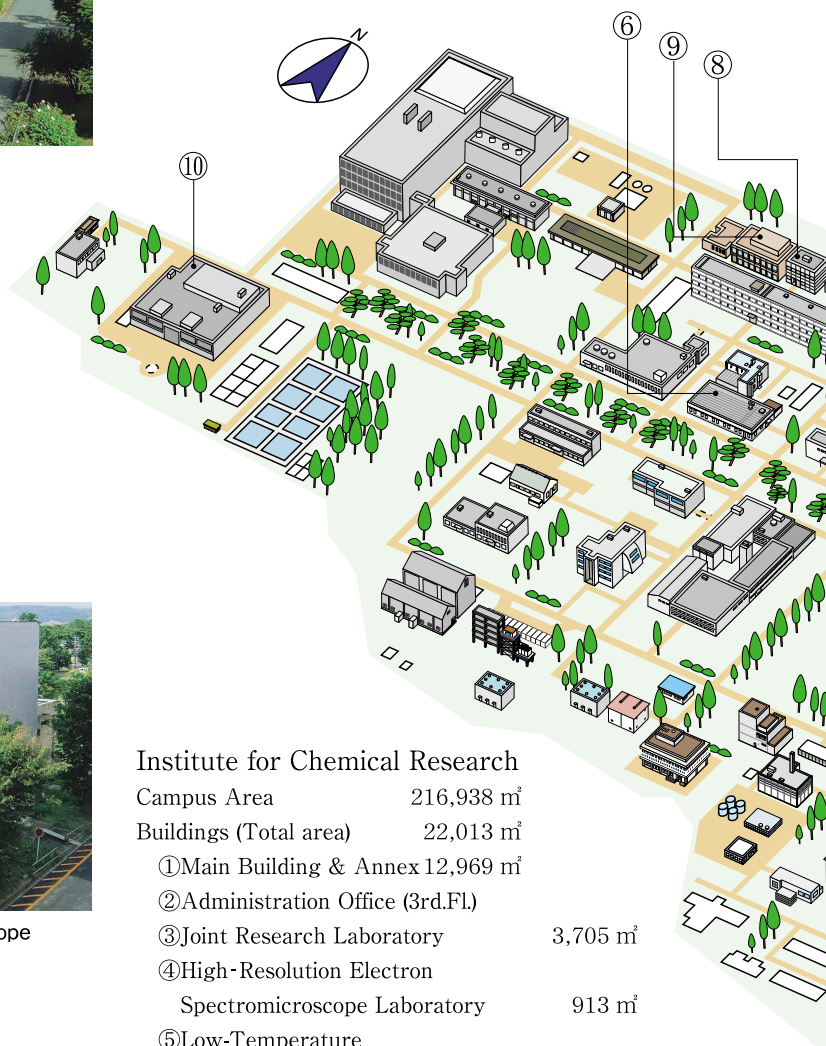
⑩ Accelerator Laboratory



④ High-resolution spectromicroscope Laboratory



Drainage Monitor Center of Uji Campus



Institute for Chemical Research

Campus Area 216,938 m²

Buildings (Total area) 22,013 m²

① Main Building & Annex 12,969 m²

② Administration Office (3rd Fl.)

③ Joint Research Laboratory 3,705 m²

④ High-Resolution Electron Spectromicroscope Laboratory 913 m²

⑤ Low-Temperature High-Resolution Electron Microscope Laboratory 586 m²

⑥ Low-Temperature Laboratory 760 m²

⑦ Bioengineering Laboratory 540 m²

⑧ Bioinformatics Center 496 m²

⑨ Nucleic Acids Laboratory 1,207 m²

⑩ Accelerator Laboratory, Nuclear Science Research Facility 2,668 m²

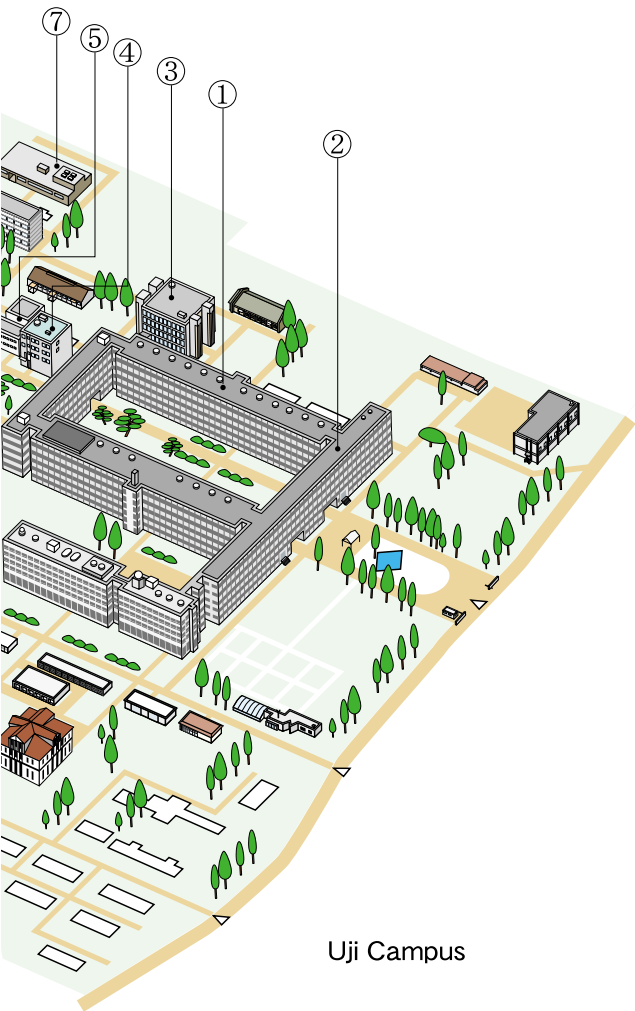


⑧ Bioinformatics Center

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.



⑨ Nucleic Acids Laboratory



Uji Campus



⑦ Biotechnology Laboratory

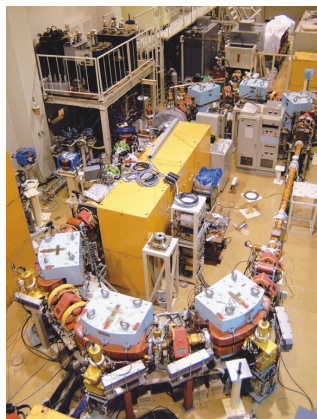


③ Joint Research Laboratory

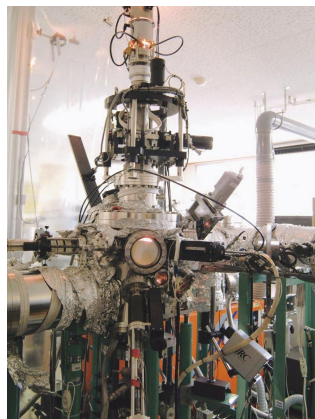
Major Research Instruments



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 Genome Net Service.



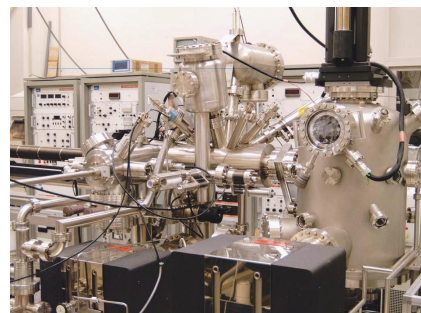
Genome Net Server(SUN Fire 15K server systems)



High-Pressure Synthesis Apparatus



Multi-Purpose Automatic Bioreactor



Photoemission Spectrometer



P3-Level Recombinant DNA Technology Laboratory



Low-Temperature Laboratory (Helium Liquefier)



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.



New Materials Development Laboratory



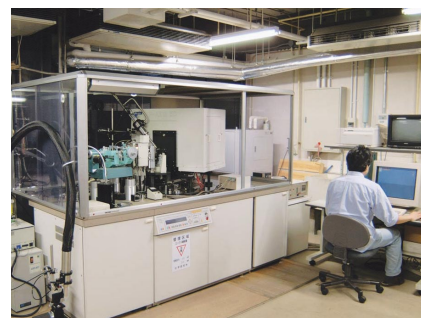
MALDI-TOF Mass Spectrometer

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 ^1H , ^{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 Diffraction System with 2-Dimensional Detector

Staff and Students

University Staff

(As Of May 1, 2002)

Professor	Associate Professor	Instructor	Sub-total	Associate Instructor	Technician	Part Timer	Sub-total	Grand Total
23 (3)	23 (3)	44	90 (6)	4	10	51	65	155 (6)

Numbers in parentheses represent visiting Professors

Graduate Students

(As of May 1, 2002)

Classification		1998	1999	2000	2001	2002
Science	Master's Course	47	40	43 (1)	57 (1)	47 (0)
	Doctoral Course	63 (6)	61 (5)	55 (4)	45 (6)	40 (3)
Engineering	Master's Course	36	33	33	38 (2)	38 (2)
	Doctoral Course	29 (2)	30 (2)	26 (3)	24 (2)	23 (5)
Agricultur	Master's Course	17 (1)	17 (2)	17 (1)	21	24 (0)
	Doctoral Course	9 (3)	9 (2)	8 (3)	9 (5)	13 (4)
Pharmaceutical Sciences	Master's Course	17 (1)	15	16	16	14 (0)
	Doctoral Course	7 (1)	6 (1)	9	9 (1)	10 (0)
Medicine	Master's Course	0	0	0	0	0
	Doctoral Course	3 (1)	3 (2)	4 (3)	3 (2)	2 (2)
Informatics	Master's Course	—	—	—	—	6 (2)
	Doctoral Course	—	—	—	—	1 (0)
Total	Master's Course	117 (2)	105 (2)	109 (2)	132 (3)	129 (4)
	Doctoral Course	111 (13)	109 (12)	102 (13)	90 (16)	89 (14)
Total		228 (15)	214 (14)	211 (15)	222 (19)	218 (18)

Figures in parentheses represent the number of foreign students

Origins of Graduate Students

(As of May 1, 2002)

University		Master's Course	Doctoral Course	Sub-Total	
Domestic	Kyoto University	67	28	95	
	Other Universities	58	47	105	
	Sub-Total	125	75	200	
Region	Country	Master's Course	Doctoral Course	Sub-Total	
Foreign	Asia	China, P. R.		3	3
		Indonesia	1	1	2
		Nepal	1		1
		Korea, R.	2	5	7
		Malaysia		1	1
		Mongolia		1	1
		Thailand		2	2
		Morocco		1	1
		Sub-Total		4	14
Total		129	89	218	



Other Research Students, Fellows and Associates

(As of May1, 2002)

	Research Student	Research Fellow	Postdoctoral Fellow of JSPS	Other Research Associate	Total
1998	6	7	5	6	24
1999	6	4	2	10	22
2000	16	5	7	14	42
2001	8	4	8	5	25
2002	7	1	3	7	18

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

Finances

(ten thousands yen)

	Personel	Non-Personel	Grants-in-Aid for Scientific Research	Contact Research	Donation for Research	Total
1997	1,261,814	1,537,829	766,400	44,764	70,052	3,680,859
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*	78,062	4,407,822
2001	1,397,585	1,725,272	795,105	356,231*	106,478	4,380,671

*For 2000, including other competitive research funds of the Japanese Government (308,796)

*For 2001, including other competitive research funds of the Japanese Government (315,230)

Major Grants and Funds in 2001(over ten million yen)

Grants-in-Aid for Scientific Research

COE Formation Basic Research Elements Science: Construction of Organic and Inorganic Frameworks Focusing on Quality of Elements	TAMAO, Kohei
Priority Areas Research (B) (1) Study on Quantum Phase Separation in the Transition Metal Oxides with Strongly Correlated Electrons	YAMADA, Kazuyoshi
Priority Areas Research (B) (2) Construction and Characterization of Composite Biocatalysts	ESAKI, Nobuyoshi
Role of Polymers for Constructing all Solid-state Ionic Devices	KOHJIYA, Shinzo
Preparatory Process Mechanism of Polymer Crystallization	KAJI, Keisuke
Priority Areas Research (C) (2) Construction and Retrieval of Highly Integrated Biological Databases	GOTO, Susumu
University and Society Collaboration Development of Order-made Artificial Restriction Enzyme and Artificial Repressor	SUGIURA, Yukio
Specially Promoted Research (2) Search for Dark Matter Axions	MATSUKI, Seishi
Scientific Research (A) (2) Elucidation of Photochemical Reactivity in Glass -an Approach from Electronic and Vibrational Structures-	YOKO, Toshinobu
Scientific Research (B) (2) Single Crystal Growth of the Oxychloride Superconductor at High Pressures and Investigation of the Physical Properties	AZUMA, Masaki
Studies on Mechanisms of Noncatalytic Elementary Organic Chemical Reactions in Super-and Subcritical Water	NAKAHARA, Masaru
Direct Observation of Polymer Network Structure by Transmission Electron Microscopy	KOHJIYA, Shinzo
Dynamism of Transformation of Active Selenium Species: Structural Biology of Mechanism of Selenoprotein Synthesis	ESAKI, Nobuyoshi
Substantiation of the Occurrence of A Diglycoside-specific Glycosidase Family in Plant Kingdom	SAKATA, Kanzo

Contact Research (Other Competitive Research Funds of the Japanese Government)

Japan Society for the Promotion of Science (JSPS) Biological Systems Database (KEGG) and Genome Information Science	KANEHISA, Minoru
Control of Magnetic Properties of Nanoscale Magnet by Structural Engineering	MIBU, Ko

Special Coordination Fund of the Ministry of Education, Culture, Sports, Science, and Technology of Japan

Hierarchy of Transcriptional Controls in Plant Signal Transduction	OKA, Atsuhiko
Computational and Experimental Analysis for Reconstruction of Genetic and Molecular Networks	KANEHISA, Minoru

Joint Researches with Nongovernment Organization

Japan Science and Technology Corporation (JST) Deductive Database of the Genome and the Biological System Based on Binary Relations	KANEHISA, Minoru
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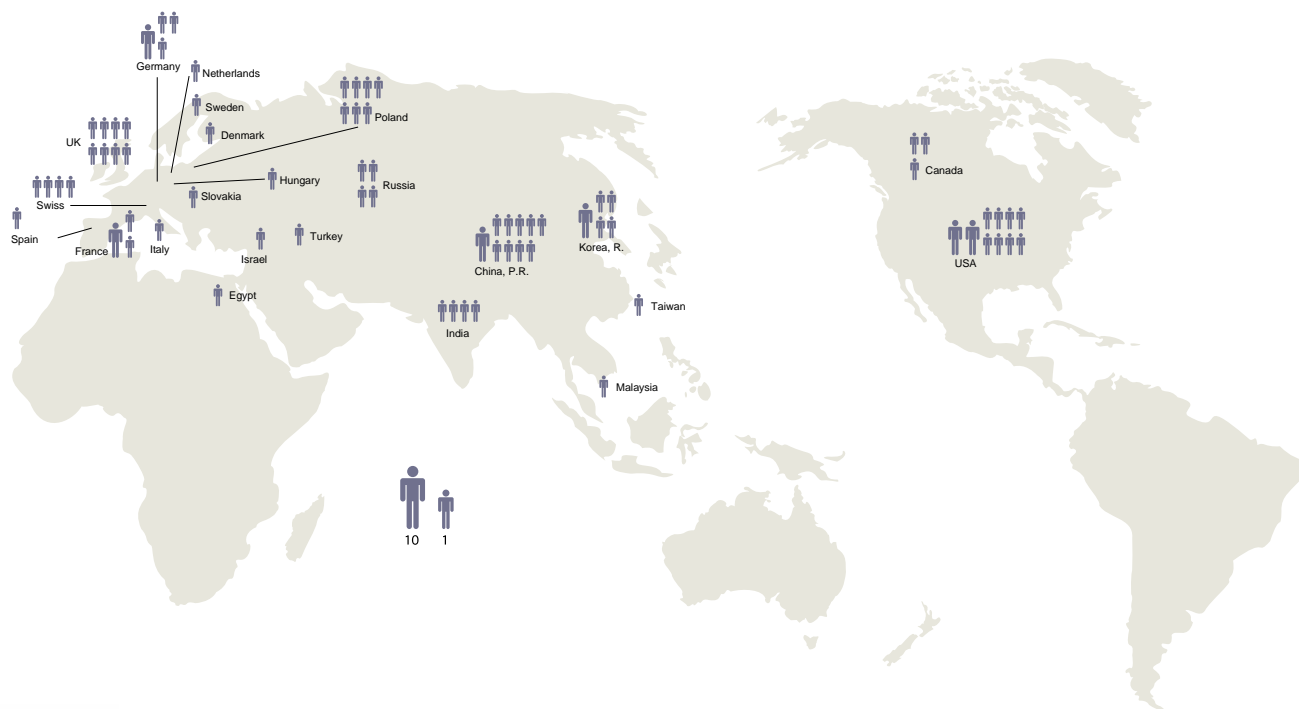


Research Activities

Publications

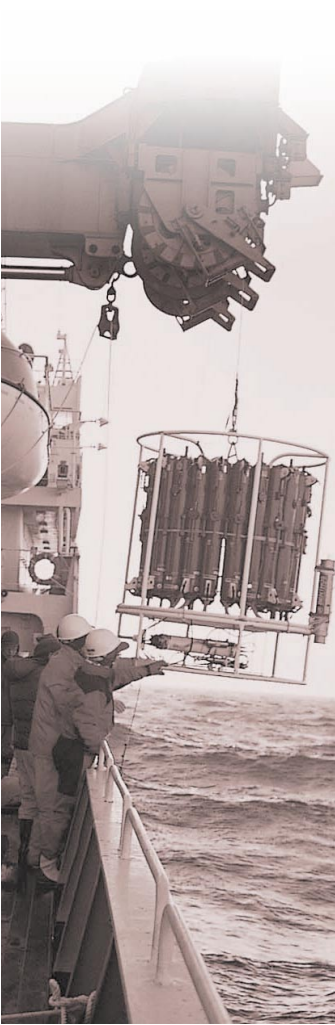
1996	1997	1998	1999	2000	2001
399	397	430	465	390	407

Visitors from foreign countries in 2001 128 people from 23 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 Chemistry; 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 for the Present Staff (the last 8 years)

1995	KAWABATA, Takeo YOSHIMURA, Tohru	The Pharmaceutical Society of Japan Award for Young Scientists Japan Society for Bioscience, Biotechnology, and Agrochemistry Award for the Encouragement of Young Scientists
1996	TSUJI, Masaki YOSHIMURA, Tohru	The Society of Fiber Science and Technology, Japan Prize for Excellence in Fiber Research The Morinaga Hoshi-kai Award
1997	SHINJO, Teruya TAKANO, Mikio TERASHIMA, Takahito FUTAKI, Shiroh	The Magnetics Society of Japan Award Society of Non-Traditional Technology, The Superconductivity Science and Technology Award Society of Non-Traditional Technology, The Superconductivity Science and Technology Award The Japanese Peptide Society Award for Young Scientists
1998	MIBU, Ko HIRAI, Asako KOMATSU, Koichi FUJI, Kaoru TOKITOH, Norihiro FUTAKI, Shiroh UEDA, Kunihiro	The Magnetics Society of Japan Young Researchers of the Year (Takei Award) The Cellulose Society of Japan Award The Divisional Award of The Chemical Society of Japan The Pharmaceutical Society of Japan Award Japan IBM Science Award The Pharmaceutical Society of Japan Award for Young Scientists Shibata Susumu Memorial Award of the Clinical Pathology Research Foundation
1999	MORIGUCHI, Sakumi KAJI, Hironori TAMAO, Kohei YAMAGUCHI, Shigehiro HIRATAKE, Jun MIYANO, Satoru	The Japanese Society for Electron Microscopy, Award for the Outstanding Technologist Award for Encouragement of Research in Polymer Science, The Society of Polymer Science, Japan The Chemical Society of Japan Award The Society of Silicon Chemistry, Japan Award for Young Chemists The Japan Bioscience, Biotechnology, and Agrochemistry Society Award for the Encouragement of Young Scientists Japanese Society for Artificial Intelligence Research Promotion Award
2000	SHINJO, Teruya URAYAMA, Kenji INOUE, Tadashi KAWACHI, Atsushi SUGIURA, Yukio	Medal of Honor with Purple Ribbon Award for Encouragement of Research in Polymer Science, The Society of Polymer Science, Japan The Society of Rheology, Japan, Research Award The Society of Silicon Chemistry, Japan Award for Young Chemists The Pharmaceutical Society of Japan Award
2001	MURAKAMI, Syozo MATUBAYASHI, Nobuyuki UCHINO, Takashi TAKAHASHI, Masahide OSAKI, Kunihiro KAWACHI, Atsushi	The Chemical Society of Japan Award for Technical Achievements Helmholtz Award, International Association for the Properties of Water and Steam Vittorio Gottardi Prize, International Commission on Glass The Ceramic Society of Japan, Young Scientists Award The Society of Rheology, Japan, Award The Chemical Society of Japan Award for Distinguished Young Chemists
2002	AZUMA, Masaki KANAYA, Toshiji TAMAO, Kohei TAMAO, Kohei YAMAGUCHI, Shigehiro	Japan Society of Powder and Powder Metallurgy Award for Innovatory Research The Society of Fiber Science and Technology, Japan Prize for Excellence in Fiber Research The 42nd Toray Science & Technology Prize (2002) (Toray Science Foundation) Frederic Stanley Kipping Award 2002, The American Chemical Society The Chemical Society of Japan Award for Distinguished Young Chemists



Educational and Social Activities

Theses

	Science	Engineering	Agricultural	Medical Sc	Pharmaceutical Sc	Total
2000	11	9	4	0	2	26
2001	13	17	1	1	2	34

Lectures

(April 1, 2001 - March 31, 2002)

2001	June 16	8th Public Lectures "A Challenge to Science with the Cosmoses, Environments, Life, and Materials"
	August 22	4rd Chemistry for High School Students - Lectures and Open Laboratories "Hear, See and Enjoy the Frontiers of Chemistry"
	October 6	5th Open Campus Uji 2001 (collaboration)
	December 7	101th Annual Symposium of Institute for Chemical Research
2002	February 22	Symposium of Graduate Students

Publications

(April 1, 2001 - March 31, 2002)

ICR Annual Report 2001, vol. 8
Profiles of Institute for Chemical Research 1926~2001 [The 75th Anniversary of Foundation] (in Japanese)
Obaku (News Letter of Institute for Chemical Research, in Japanese), No. 15, 16

Web Pages

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

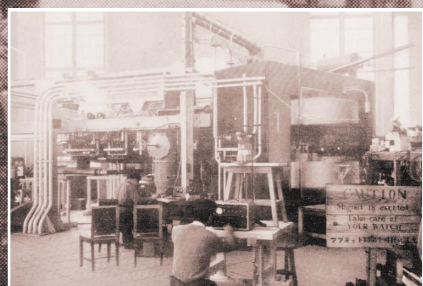
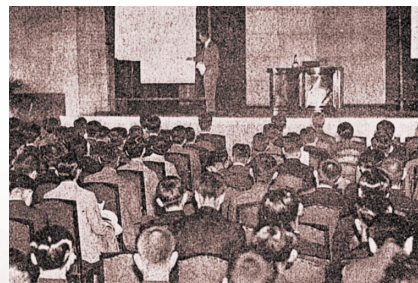


Committee on Public Relations / YAMADA, Kazuyoshi AKUTSU, Tatsuya
TAMAOKohei
Desk for Administration Department / NAGASAKI, Junichi MIYAMOTO, Mariko
KOBAYASHI, Sayuri NISHIMURA, Maki
Public Relations Section / UENOYAMA, Mika KARIKOMI, Miwako



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	TAKEL, 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			





The Institute For Chemical Research Kyoto University

Gokasho,Uji,Kyoto,611-0011 Tel.0774-38-3344 Fax.0774-38-3014
URL http://www.kuicr.kyoto-u.ac.jp/index_1.html



Location and Transportation

- From Obaku Station on the Keihan Uji Line: 6 min by walk
(from Keihan-Sanjo Station to Obaku Station: 35 min)
- From Obaku Station on the JR Nara Line: 5 min by walk
(from Kyoto Station to Obaku Station: 20 min)
- From Kyoto-Minami Interchange: 25 min by car
- From Uji-Higashi Interchange: 5 min by car