

# Department of Macromolecular Science

Macromolecular Science was born in the middle of the last century and made rapid progress in the last several decades to fill the gap between traditional disciplines and to meet the practical needs of the new era. However, macromolecular science is not a mere extension of chemistry or physics but stands at the crossroads of chemistry, physics, and life science. Especially, macromolecular science has been regarded as an important field of science for understanding of biological phenomena at a molecular level. Macromolecules are known as a typical complex system and have recently attracted the great interest of many scientists in the field of physics. Thus, macromolecular science must be one of the most important fields of natural science in this new century.

There are several universities having departments of macromolecular science in Japan. However the department of macromolecular science of Osaka University is unique in the sense that it belongs to the graduate school of science. The others belong to the faculty of engineering, aiming at practical applications. This indicates that the objective of our department is basic research on macromolecules. The department consists of four major research groups: there are a total of ten laboratories covering major subjects of the macromolecular science as described below. The staffs of each laboratory are famous over the world.

The department is active in international exchange. Many leading scientists of macromolecular science visit our department. The department organizes the international symposium named as "Osaka University Macromolecular Symposium" (OUMS) every two or three years. Of course there are many foreign students.

The macromolecular science course devotes itself to training graduate students by offering a systematic lecture course in macromolecular chemistry and physics. It also guides students by making them engaged in basic researches at one of the ten laboratories. Through their graduate studies, students acquire various professional knowledge and techniques leading to the degrees of the master or doctor of science.

## Research Group of Polymer Synthesis and Reaction Chemistry

In order to create new polymer materials with special functions and/or excellent properties, similar to biopolymers, the Laboratory of Polymer Synthesis aims to investigate new ideas and methods which allow us to control the structure and the molecular weight of these polymers in a precise manner. For example, this group could find out the highly selective living polymerization system with no side reactions through the research on the cationic polymerization reaction mechanism. As a result, it is now possible to produce various types of polymers such as polymers with homogeneous chain length and structure, polymers with special shape or unique properties, polymers which are highly sensitive to external stimulus, etc.

In the Laboratory of Macromolecular Reaction Chemistry, a wide variety of studies on syntheses and functionalization of macromolecules has been done based on macromolecular science, coordination chemistry and organometallic chemistry. Unique reactivity of metal complexes is applied to development of a new polymerization catalyst and precise design of macromolecular complexes. Metalloenzyme can be recognized as a representative example of functional biomacromolecules incorporating metal complexes. To understand the mechanism of metalloenzyme function, synthesis and structural characterization of a model of active

site and non-natural peptides are investigated.

## Research Group of Structure, Function, and Properties of Polymers

Polymer chain molecules have a large number of the internal degrees of freedom and sometimes form higher-order structures. They can easily respond to the change of external fields such as mechanical and electric fields by changing their internal structures. This is a common feature of "soft matters" including micelles, liquid crystals, supramolecules, and so on. The laboratory of Polymer Physical Chemistry investigates physicochemical and rheological properties of the soft matters through viscoelastic, dielectric, rheo-optical, and nuclear magnetic resonance relaxation measurements in order to elucidate the nature of macromolecules.

Molecular recognition by macromolecules plays an important role, for example, in substrate specificity of enzymes and antigen-antibody reactions in human life. Selective molecular recognition among macromolecules is achieved through a large number of weak interactions. The Laboratory of Supramolecular Functional Chemistry constructs functionalized sensing, catalytic, and energy conversion systems by utilizing monoclonal antibodies. We also create stimuli-responsive and self-healing materials based on molecular recognition of cyclodextrins or hybridization of bio-related macromolecules with synthetic molecules.

Synthesis of macromolecules with well-defined chemical structures (i.e., precise macromolecules) has been one of important challenges in macromolecular science. The Laboratory of Macromolecular Precise Science strives to construct a new type of precise macromolecules with specific primary structures. Various properties of these precise macromolecules, e.g., hydration and association properties, are investigated to understand the nature of macromolecules (i.e., macromolecularity) in more detail. This laboratory also aims at creation of high-performance macromolecules comparative to biological macromolecules using the precise macromolecules.

## Research Group of Macromolecular Assemblies

Any small change in the primary structure may lead to some serious effect on its higher structural hierarchy. For example, lack of vitamin C causes the fatal disease "scurvy" because that stops formation of normal collagen fiber. That is, without vitamin C, no hydroxylation of proline takes place and thereby no further stabilization of collagen fiber. The Laboratory of Macromolecular Structure aims to elucidate the relationship between structure and physical properties (or functions) of macromolecules at atomic resolution using X-ray diffraction, neutron scattering and infrared and Raman spectroscopy.

Polymers bearing functional groups of strong attractive interactions like the hydrophobic and ionic interactions as well as hydrogen bonding form various types of polymer aggregates to exhibit unique properties and functions. Basic understanding of these polymers is important in the fields not only of polymer industry but also of molecular biology. The Laboratory of Polymer Assemblies investigates interrelation among the chemical structure, self-associating structure, and properties of polymer aggregates in solution. Currently this laboratory studies amphiphilic polyelectrolytes, intra- and intermolecularly hydrogen-bonding polymers, polymer living anions, helical polymers, and so on.

## Research Group of Informative Polymer Science

**Laboratory of Protein Folding:** Protein folding is a process in which an extended polypeptide chain acquires a unique folded conformation with biological activity. Laboratory of Protein Folding is investigating the mechanism of protein folding and misfolding to improve our understanding of the structure and function of proteins. This topic is also important for understanding of many critical biological processes and disease states because these involve protein misfolding such as amyloid fibril formation. We are studying the mechanism of protein folding and misfolding with various approaches including spectroscopies (NMR, fluorescence, CD), physicochemical measurements (calorimetry, analytical ultracentrifugation) and fluorescence microscopy.

**Laboratory of Protein Crystallography:** In 1959 the lab was established as the division of Protein Crystallography to elucidate the molecular structure of proteins by X-ray crystallography. Nowadays the X-ray method has become the most powerful tool to determine protein structures. One of our aim is to spread the application of this method throughout biological science. Current research projects are focused on biological macromolecular assemblies and membrane proteins. Especially, our lab is interested in studying the structure and function of biological energy transducing proteins, such as photosynthetic electron transfer complex and microtubule dynein motor.

The aim of the Laboratory of Supramolecular Crystallography is to elucidate the structure of biological macromolecules and biological macromolecular assemblies to understand their functions based on the atomic structures. X-ray crystallography is one of the most powerful tools for structure determination of biological macromolecules and biological macromolecular assemblies, and we are also working on the development of new technologies and methodologies of protein crystallography, including the synchrotron radiation beamline at SPring-8.

**Laboratory of Chemistry for Environment and Safety:** Li ion battery has now become a fundamental device in our daily life. However, the use of organic solvents and very high energy density in Li ion batteries introduce the battery include dangerous hazards such as ignition accidents. In this laboratory, we are developing a new class of solid polymer electrolytes, named low-barrier ion conductive polymer electrolytes, for Li ion batteries to realize the safety of these batteries. In addition, this laboratory aims at developing new photo-chemical energy conversion system. As the laboratory belongs to the department for the administration of safety and hygiene, we carry out the research projects to contribute to the safety of science and technology, together with the activity for maintaining the safety level of university research work and experiments.

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# Laboratory of Polymer Synthesis

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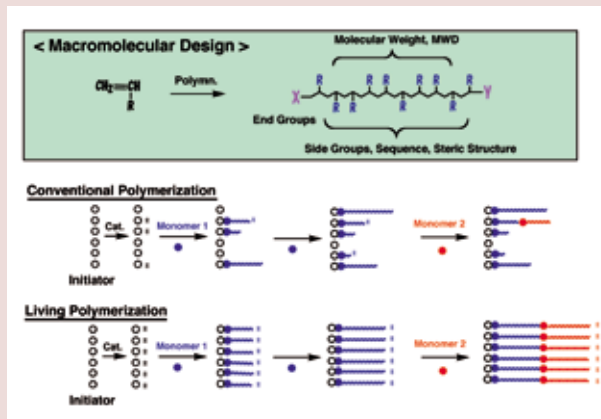
**Home Page** [http://www.chem.sci.osaka-u.ac.jp/lab/aoshima/e\\_index.html](http://www.chem.sci.osaka-u.ac.jp/lab/aoshima/e_index.html)

## [Research Projects]

Recently, well-designed stimuli-responsive polymers have attracted much interest as precursors of advanced polymer materials such as nano-organized self-assemblies, intelligent hydrogels, and DDS. In particular, recent progress in living polymerization has encouraged us to design various types of block copolymers in order to examine their stimuli-induced self-association. We have prepared a variety of functional polymers with well-controlled structures and molecular weights by living cationic polymerization in the presence of an added base. On the basis of these results, we have designed a new strategy for preparing block copolymers with various types of stimuli-responsive properties such as thermosensitive physical gelation.

## [Research Area]

- 1) Syntheses of well-defined polymers with various characteristic properties by living cationic polymerization.
- 2) Syntheses of advanced stimuli-responsive block copolymers.
- 3) Investigation of polymerization mechanism and design of novel living polymerization.



Concept of macromolecular design and living polymerization for syntheses of well-designed stimuli-responsive polymers

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# Laboratory of Macromolecular Reaction Chemistry

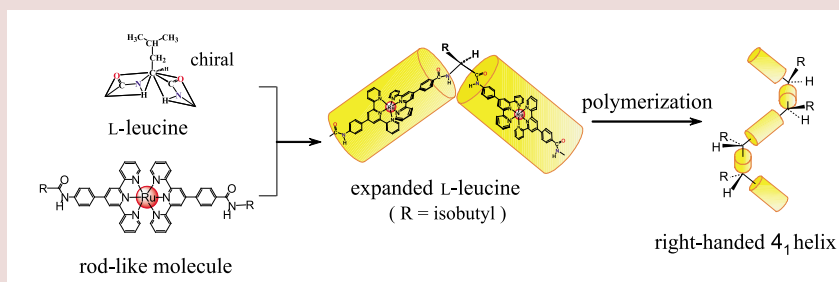
**Members** Kiyotaka ONITSUKA (Professor), Taka-aki OKAMURA (Associate Professor), Naoya KANBAYASHI (Assistant Professor)

**Home Page** <http://www.chem.sci.osaka-u.ac.jp/lab/onitsuka/en/>

## [Research Area]

Our research involves the development of new polymer synthesis and functionalization incorporating a characteristic feature of metal elements. For example, precise design of new transition metal complexes and investigation of their reactivity lead to the development of new polymerization catalysts. Functionalization of polymers based on the control of molecular structure is investigated by using the methodology of organic synthesis. Our research interest is also focused on metalloenzyme. Model complexes of active sites and non-natural peptide are designed and structurally characterized.

- 1) Development of new organometallic polymerization catalysts and their application to synthesis of functional polymers
- 2) Functional macromolecular complexes composed of organometallic units
- 3) Investigation of the reactivity controlling mechanism in the active center of metalloenzyme using model complexes having simple ligands and/or short peptides.
- 4) Synthesis of non-natural amino acid polymers for higher order structure formation and expression of novel functions.



## Laboratory of Polymer Physical Chemistry

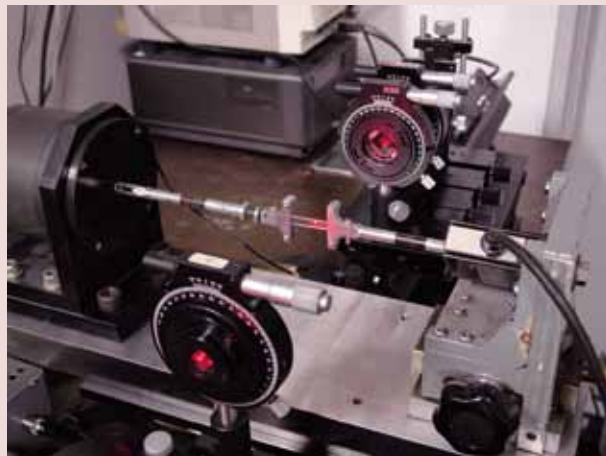
**Members** Tadashi INOUE (Professor), Osamu URAKAWA (Associate Professor), Takuya KATASHIMA (Assistant Professor)

**Home Page** [http://www.chem.sci.osaka-u.ac.jp/lab/inoue/index\\_e.html](http://www.chem.sci.osaka-u.ac.jp/lab/inoue/index_e.html)

### [Research Projects]

- 1) Shear induced structures of soft matters.
- 2) Nonlinear rheology and rheo-optics of polymer solids.
- 3) Molecular motions of hyper-branched polymers.
- 4) Structure and molecular motions of supramolecules.
- 5) Hydration and molecular motions of water-soluble polymers.
- 6) Structure and dynamics of polymer composites.

Soft matter stands for soft materials including polymers, liquid crystals, suspensions, and self-assembling molecules which form a large mesoscopic structure much larger than atoms. Soft matters are “soft” and therefore they can easily respond to external fields like strain fields, flow fields, electric fields and so on, and sometimes show drastic structural changes. We have been studying their unique physicochemical properties, particularly nonlinear responses under strong external fields, in addition to their fruitful equilibrium properties and dynamics. Our research is focused on molecular interpretation of rheological phenomena of polymers and micelles as a model system of soft matter.



## Laboratory of Supramolecular Functional Chemistry

**Members** Hiroyasu YAMAGUCHI (Professor), Yoshinori TAKASHIMA (Associate Professor)

**Home Page** <http://www.chem.sci.osaka-u.ac.jp/lab/yamaguchi/english/index.html>

### [Research Projects]

- 1) Preparation of functionalized supramolecular complexes using host molecules such as cyclodextrins or monoclonal antibodies.
- 2) Creation of stimuli-responsive and self-healing materials based on self-assembly of bio-related and/or synthetic molecules.
- 3) Development of a high performance sensing element.
- 4) Construction of energy conversion and catalytic systems using hybrids of biomacromolecules with synthetic molecules.

In biological systems, life processes are led by the unique behavior of macromolecules such as proteins and DNA. Molecular recognition by macromolecules plays an important role, for example, in substrate specificity of enzymes and antigen-antibody reactions in human life. Selective molecular recognition among macromolecules is achieved through a large number of weak interactions. We have focused our attention on molecular recognition events of host molecules such as cyclodextrins and monoclonal antibodies. In this laboratory, we create unique supramolecular complexes or novel materials through molecular

recognition of these molecules or hybridization of bio-related macromolecules with synthetic molecules. Functionalized sensing, catalytic, and energy conversion systems are also constructed.





## Laboratory of Macromolecular Precise Science

**Members** Akihito HASHIDZUME (Professor)

**Home Page** [http://www.chem.sci.osaka-u.ac.jp/lab/hashidzume/index\\_eng.html](http://www.chem.sci.osaka-u.ac.jp/lab/hashidzume/index_eng.html)

Macromolecular substances are ubiquitous, and these substances enrich our lives. Our bodies are also composed of macromolecules, e.g., nucleic acids and proteins. To unravel the reasons behind why life has chosen macromolecules as essential building blocks, and to elucidate the crucial roles that macromolecules play in our life, we devote our efforts to understand the nature of macromolecules, i.e., macromolecularity using precise macromolecules. We also aim at the creation of high-performance macromolecules based on macromolecularity. We are thus carrying out the following three projects.

### [Research Projects]

#### 1) Creation of Precise Macromolecules

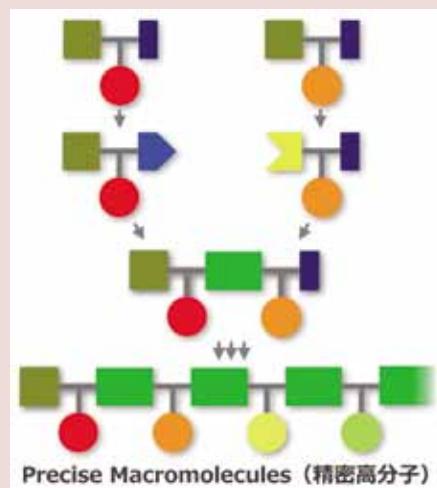
We synthesize precise macromolecules with well-defined chemical structures because these precise macromolecules are critical for deeper understanding of macromolecularity.

#### 2) Understanding of Macromolecularity

We strive to understand macromolecularity utilizing the precise macromolecules.

#### 3) Creation of High-Performance Macromolecules

We challenge existing boundaries to creation of high-performance macromolecules comparative to biological macromolecules using the precise macromolecules.



## Laboratory of Macromolecular Structure

**Members** Katsumi IMADA (Professor), Fumitoshi KANEKO (Associate Professor), Tatsuya KAWAGUCHI (Assistant Professor)

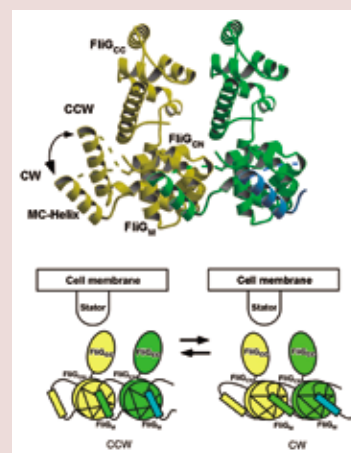
**Home Page** <http://www.chem.sci.osaka-u.ac.jp/lab/imada/en/index.html>

### [Research Area]

Biological process is driven by complex molecular machines composed of biological macromolecules. The flagellum, which is an organelle for bacterial motility, is one of those molecular machines. The flagellum is a huge protein assembly composed of a helical filamentous screw, a molecular universal joint, a highly efficient ion-driven motor and a protein export apparatus for self-construction. The Laboratory of Macromolecular Structure aims to provide fundamental understanding of operating principles and the self-assembly mechanism of biological macromolecular machines, such as the bacterial flagellum, through the studies of molecular structure at atomic resolution and reconstitution of the molecular machines. We also study structures of polymer complexes with low molecular weight compounds and the relationship between their structures and functions.

- 1) Rotational mechanism of the bacterial flagellar motor.
- 2) Self-assembly mechanism of the bacterial flagellar motor.
- 3) Structural and functional studies on bacterial protein secretion systems

- 4) Structural and functional studies on environmental sensing units of bacteria.
- 5) Study on the structure of polymer complex with small molecule and its formation mechanism.



A plausible model for rotational switching in bacterial flagella.

## Laboratory of Polymer Assemblies

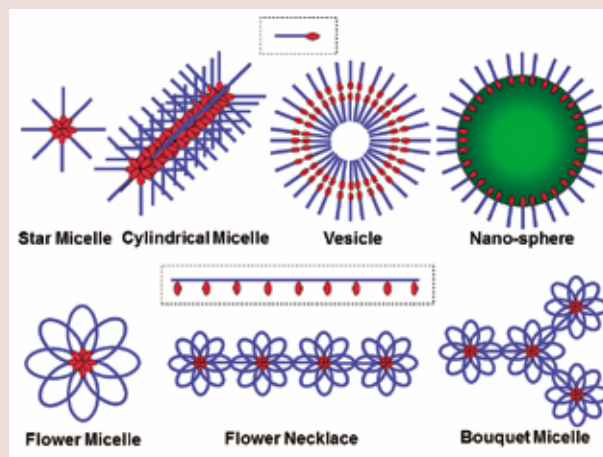
**Members** Takahiro SATO (Professor), Ken TERAOKA (Associate Professor)

**Home Page** <http://osku.jp/k072>

Polymers often form aggregates in solution and polymer aggregates play important roles in industries of foods, cosmetics, paints, and pharmaceuticals, as well as in living cells where proteins and nucleic acids associate and dissociate during biochemical reactions. Polymer aggregates, or polymer assemblies, usually take very complex conformations and their characterization is not easy. Our group aims at understanding the structures and properties of polymer assemblies through the following projects.

### [Research Projects]

- 1) Polymer micelles formed by amphiphilic polymers.
- 2) Polymer complexes formed by amphiphilic polymers and various substances
- 3) Polyion complexes formed by oppositely charged polyelectrolytes
- 4) Conformation and molecular recognition of polysaccharides
- 5) Molecular conformation and liquid crystallinity of cyclic and branched polymers



## Laboratory of Protein Folding

(Institute for Protein Research)

**Members** Yuji GOTO (Professor), Young-Ho LEE (Associate Professor), Masatomo SO (Assistant Professor)

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### [Current Research Programs]

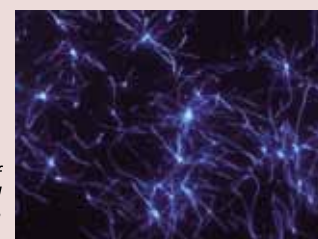
- 1) Observation of folding processes and clarification of the mechanism of protein folding.
- 2) Analysis of structural stability and dynamics of protein molecules.
- 3) Analysis of structural stability and the mechanism of formation of amyloid fibrils.

Protein folding is a process in which an extended polypeptide chain acquires a unique folded conformation with biological activity. However, the exact molecular mechanism remains unknown. Clarifying the mechanism of protein folding is essential to improve our understanding of the structure and function of proteins. It is also important to design engineered proteins with improved functions.

Moreover, protein folding plays important roles in many biological phenomena. For an example, the deposition of amyloid fibrils has been suggested to play a central role in over 20 degenerative disorders including Alzheimer's and prion diseases. Because the amyloid fibril deposition is often caused by misfolding

of an originally functional protein, these diseases are called "folding disease". In order to establish therapeutic treatments, clarifying the molecular mechanism of folding diseases is essential.

We are studying the conformational stability of proteins, molecular basis of folding reaction, and structures and formation of amyloid fibrils. These studies are performed using various observation methods, including spectroscopies (NMR, CD, IR), physicochemical methods (calorimetry, ultracentrifugation), and fluorescence microscopy, as well as gene manipulations for recombinant proteins by using the *E.coli* and yeast expression systems.



An image of amyloid fibrils of amyloid- $\beta$  peptide obtained using total internal reflection fluorescence microscopy.

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## Laboratory of Protein Crystallography

(Institute for Protein Research)

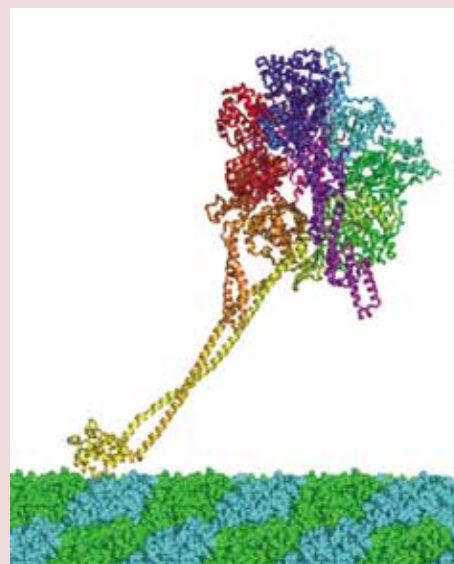
**Members** Genji KURISU (Professor), Hideaki TANAKA (Associate Professor),  
Naoko NORIOKA (Technical Assistant)

**Home Page** <http://www.protein.osaka-u.ac.jp/crystallography/EngHP/>

### [Research Interests]

- 1) Structural studies of photosynthetic energy-transducing membrane protein complex and related redox enzymes
- 2) Crystal structure analyses of dynein motor
- 3) Damage-free crystal structure analysis of metalloproteins at high resolution

Three-dimensional protein structure brings us a deeper insight into the biological function. X-ray crystallography is the best method to determine atomic coordinates of protein molecules. The main aim of our group is the X-ray structure determination of the biological macromolecular assemblies including membrane protein complexes, in order to elucidate the molecular mechanism of the highly organized biological processes at atomic level.



Crystal Structure of the dynein motor domain

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## Laboratory of Supramolecular Crystallography

(Institute for Protein Research)

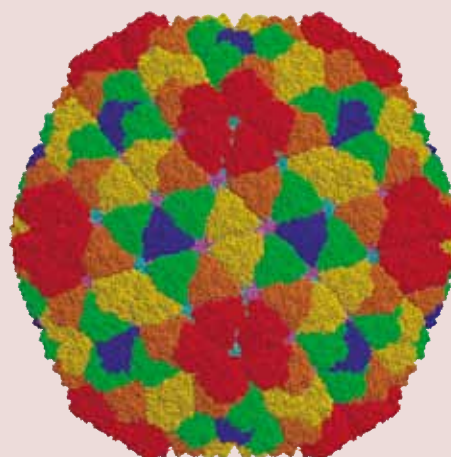
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Kohei TAKESHITA (Specially Appointed Assistant Professor),  
Hirotaka NARITA (Specially Appointed Assistant Professor)

**Home Page** <http://www.protein.osaka-u.ac.jp/rcsfp/supracryst/en/>

### [Current Research Projects]

- 1) X-ray structure determination of biological macromolecular assemblies and proteins.
- 2) Development methodologies for X-ray structure determination of biological macromolecular assemblies using synchrotron radiation and X-ray free electron laser.
- 3) Development of data processing algorithm of diffraction data from micro-crystals.

Macromolecule assemblies, consisting of proteins, nucleic acids, and other substances, play key roles in all living system. Our laboratory works on structure determination of biological macromolecular assemblies using X-ray diffraction technique. Development of tools for X-ray crystallography of biological macromolecular assemblies, including the synchrotron radiation beamline at SPring-8, is also one of our main works.



# Laboratory of Chemistry for Environment and Safety

(Department for the administration of safety and hygiene)

**Members** Hitoshi YAMAMOTO (Professor), Hideki MOMOSE (Associate Professor)

**Home Page** <http://www.osaka-u.ac.jp/jp/facilities/anzen/kankyoku/>

## [Research Projects]

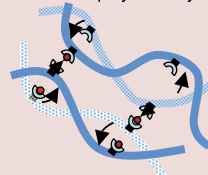
- 1) Development of low barrier ion conductive polymer electrolytes.
- 2) Development of the photo-switching functional molecules.
- 3) Development of detection methods for environmental chemicals.
- 4) Construction of education system for realization of safety conscious culture in the university.
- 5) Research and analyses of university accidents in the world.

This laboratory belongs to the department for the administration of safety and hygiene, whose mission is managing safety and hygiene of all people constituting the university. The research in this laboratory aims to contribute to the safety of wide area in science and technology.

At present, our research projects focus on development of new functional molecules such as low barrier ion conductive polymers for the safety of Li ion batteries, photo-switchable hydrogen bonds for environmental chemistry, etc.

In addition, our laboratory proposes safe methods and techniques for conducting research and experiments through investigation and analyses of university accidents in the world.

Conventional polyelectrolytes



Li ion transfer based on the segment motion

Activation energy  $> 40 \text{ kJ/mol}$

Low-barrier polyelectrolytes



Li ion transfer based on the single bond rotation

Activation energy  $< 7 \text{ kJ/mol}$

