Department of Macromolecular Science

# 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 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 the 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 twelve laboratories covering major subjects of 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 "Osaka University Macromolecular Symposium" (OUMS) every two or three years. Of course, there are many international 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 research 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 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 micellae, liquid crystals, supramolecules, and so on. The laboratory of Polymer Physical Chemistry investigates physicochemical and rheological properties of 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 antigenantibody 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.

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.

Macromolecules have specific conformational behaviors in solution because of the high degree of freedom in the internal rotation. Various macromolecular assemblies with unique properties can therefore form in solution. The Laboratory of Macromolecular Solutions aims to investigate dilute and concentrated solution properties of macromolecules and macromolecular assemblies. Light and X-ray scattering methods, solution viscosity, and various spectroscopies are combined to elucidate the origin of the molecular conformation in solution as well as the mechanism to form macromolecular assemblies. Intermolecular interactions and thermodynamics of macromolecular solutions are also investigated to clarify the relationship between the conformation and the phase behavior.

#### Research Group of Informative Polymer Science

The aim of the Laboratory of Cryo-EM Structural Biology is to clarify the mechanisms of molecular machines based on the structural analysis by cryo-EM. The cryo-EM is one of the structural analysis methods, that has been drawing attention in recent years, and we are developing high-resolution structural analysis methods and techniques. We are elucidating the energy conversion mechanism of molecular motors and analyzing the structure of olfactory receptors by using these technologies.

Laboratory of Protein Crystallography was established in 1959 to elucidate the molecular structure of proteins by X-ray crystallography. Nowadays the combination of X-ray and Cryo-EM technique has become the most powerful way 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.

#### Department of Environment and Safety

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.

# Institute for Advanced Co-Creation Studies

Laboratory of polymeric materials design: Tough and flexible polymeric materials are used in various manufacturing industries and healthcare applications. However, polymeric materials are brittle and easily broken when concentrated external stress is applied to the material. To enhance their mechanical strength, materials scientists have improved polymeric, we investigated innovative polymeric materials design using host-guest interactions between cyclodextrin (CD) and hydrophobic guest molecules via supramolecular reversible bonds. We found a variety of supramolecular polymeric materials, such as macroscopic self-assemblies, self-healing materials, artificial muscles, and shape memory materials. We prepared tough and flexible bulk polymeric materials by using various hydrophobic acrylates modified with CD hosts or guests. The obtained polymers have host and guest moieties as their side chains to form elastomers with high flexibility and toughness.

#### Home Page

http://www.chem.sci.osaka-u.ac.jp/graduate/mms/en/index.html

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Department of Macromolecular Science	Laboratory of Polymer Synthesis	
	Members Sadahito AOSHIMA (Professor), Arihiro KANAZAWA (Associate Professor)	
	Home Page http://www.chem.sci.osaka-u.ac.jp/lab/aoshima/	

#### [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 selfassociation. 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 stimuliresponsive properties such as thermosensitive physical gelation.

#### [Research Area]

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



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

#### Department of Macromolecula Science

# 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 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
- Investigation of the reactivity controlling mechanism in the active center of metalloenzyme using model complexes having simple ligands and/or short peptides.
- Synthesis of non-natural amino acid polymers for higher order structure formation and expression of novel functions.



Department of Science Laboratory for Polymer Physical Chemistry Members Tadashi INOUE (Professor), Osamu URAKAWA (Associate Professor)

#### [Research Interests]

- 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.
- 7) Entanglement of semiflexible polymers.

The term "soft matter" stands for soft materials which form a mesoscopic structure much larger than atoms, including polymers, liquid crystals, suspension, and self-assembling molecules. Soft matters are actually "soft," and they can efficiently respond to external fields like strain fields, flow fields, electric fields, and so on. They sometimes show drastic structural changes. We have studied their unique physicochemical properties, particularly nonlinear responses under strong external fields, including their fruitful equilibrium properties and dynamics. We have focused on the molecular interpretation of rheological phenomena of polymers and micellae as a model system of soft matter.



#### Department of Macromolecula Science

# Laboratory of Supramolecular Functional Chemistry

nbers Hiroyasu YAMAGUCHI (Professor), Yuichiro KOBAYASHI (Assistant Professor)

http://www.chem.sci.osaka-u.ac.jp/lab/yamaguchi/english/index.html

#### [Research Interests]

- 1) Development of a high performance sensing element.
- Construction of energy conversion and catalytic systems using hybrids of biomacromolecules with synthetic molecules.
- Creation of functionalized supramolecular materials based on selfassembly of bio-related and/or synthetic polymers.

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 the special behavior of antibodies, especially monoclonal antibodies, because they can recognize a larger and more complex compound with high specificity. In this laboratory, we develop novel supramolecular materials and construct functionalized sensing, catalytic, and energy conversion systems via specific molecular recognition of biomacromolecules and selective assembly of bio/synthetic molecules.





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.



Precise Macromolecules (精密高分子)

Department

# Laboratory of Macromolecular Structure

Katsumi IMADA (Professor), Fumitoshi KANEKO (Associate Professor), Tatsuya KAWAGUCHI (Lecturer), Norihiro TAKEKAWA (Assistant Professor)

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 selfconstruction. 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.

- Rotation mechanism of bacterial motor systems. 1)
- 2) Self-constitution mechanism of bacterial motility machines.

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



Schematic drawing of the bacterial hook basal-body architecture



#### [Research Area]

Macromolecules in solution can take a nearly infinite number of conformations due to their high degree of freedom of internal rotations. Macromolecules in solution have, therefore, specific characteristics not found in small molecules. Intramolecular interactions in a macromolecule and intermolecular interactions with solvent molecules significantly influence the molecular shape in solution. Furthermore, strong intramolecular interactions, including hydrogen bonding and electrostatic interactions, lead to the formation of micelles and aggregates. The intermolecular interactions between polymers through solvents can also cause various phase separations. Such phenomena correlate with the functions in biosystems. Our research aim is to clarify the various phenomena exhibited by macromolecules in solution, that is, single chain conformation, complex formation behavior, and phase separation behavior by using the latest scattering and spectroscopic methods.

#### [Research Projects]

- 1) Conformation and molecular recognition ability of polysaccharides and their derivatives
- Molecular conformation and intermolecular interactions of ring and 2) branched polymers
- 3) Aggregation and phase separation of branched polymers-poor solvent systems
- 4) Complex formation of polymers with nanoparticles



#### Laboratory of CryoEM Structural Biology Department (Institute for protein research) Science Takayuki KATO (Professor), Jun-ichi KISHIKAWA (Assistant Professor), Hiroko TAKAZAKI (Assistant Professor), Mika HIROSE (Specially Appointed Researcher), Kiyo TUNEZUMI (Specially Appointed Researcher)

http://www.protein.Osaka-u.ac.jp/cryoem/index.html e Page

#### [Research Interests]

- (1) Study of energy conversion mechanism of molecular motor
- (2) Structural analysis of olfactory receptors
- (3) Study of molecular dynamics by cryo-electron microscope
- (4) Development of high-resolution structural analysis method by cryo-electron microscope

The biomolecules such as protein and nucleotide are responsible for life activity, its function is relative to the structure. In our laboratory, we will clarify the molecular mechanism by structural analysis using a cryo-EM. In particular, we are analyzing the energy conversion mechanism of motor protein such as flagellar motors and ATPase, and the mechanism of olfactory receptors. We are also developing of the method for analysis of molecular dynamics by cryo-EM and for high-resolution and high-resolution structural analysis by cryo-EM.





Cryo-EMs



#### [Research Interests]

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

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



Crystal Structure of the dynein motor domain

# Department Science

# (Institute for Protein Research) Laboratory of Supramolecular Crystallography

Atsushi NAKAGAWA (Professor), Mamoru SUZUKI (Associate Professor), Eiki embers YAMASHITA (Associate Professor)

http://www.protein.osaka-u.ac.jp/physical/ ne Page

#### [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.





- Development of low barrier ion conductive polymer electrolytes. 1)
- 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 department 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.





the single bond rotation Activation energy <7kJ/mol

# Laboratory of Polymeric Materials Design

Department Science

#### (Institute for Advanced Co-Creation Studies)

Yoshinori TAKASHIMA (Professor), Junsu PARK (Specially Appointed Assistant Professor)



#### [Research Area]

Tough and flexible polymeric materials are used in various manufacturing industries and healthcare applications. However, polymeric materials are brittle and easily broken when concentrated external stress is applied to the material. To enhance their mechanical strength, materials scientists have improved polymeric, we investigated host-guest interactions between CDs and hydrophobic guest molecules via supramolecular reversible bonds. We found a variety of supramolecular polymeric materials, such as macroscopic self-assemblies, self-healing materials, artificial muscles, and shape memory materials. We prepared tough and flexible bulk polymeric materials by using various hydrophobic acrylates modified with CD hosts or adamantane guests. The obtained polymers have host and guest moieties as their side chains to form elastomers with high flexibility and toughness.

#### **Research topics.**

- (1) Creation of polymeric materials with reversible bonding.
- (2) Creation of polymer materials with movable cross-linking
- (3) Creation of polymeric materials combining reversible and movable cross-linking.
- Creation of stimuli-responsive polymeric materials (4)
- (5) Creation of polymeric materials combining natural and synthetic polymers.

