

# Joint Studies Programs

As one of the important functions of an inter-university research institute, IMS facilitates joint studies programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and selected by an interuniversity committee.

## (1) Special Projects

### (a) Molecular Simulation on Structural Change of Tritium-Substituted Polymeric Materials by Decay from Tritium to Helium-3

FUJIWARA, Susumu (*Kyoto Inst. Tech.*)  
 MIZUGUCHI, Tomoko (*Kyoto Inst. Tech.*)  
 SAKAI, Wataru (*Kyoto Inst. Tech.*)  
 LI, Haolun (*Kyoto Inst. Tech.*)  
 NAKAMURA, Hiroaki (*NIFS*)  
 HATANNO, Yuji (*Univ. Toyama*)  
 SAITO, Seiki (*Yamagata Univ.*)  
 SAIKI, Toshiharu (*Keio Univ.*)  
 OTSUKA, Takao (*RIKEN*)  
 KENMOTSU, Takahiro (*Doshisha Univ.*)  
 ASO, Tsukasa (*Natl. Inst. Tech., Toyama College*)  
 YASUNAGA, Takuo (*Kyushu Inst. Tech.*)  
 OYA, Yasuhisa (*Shizuoka Univ.*)  
 TOGARI, Akihiro (*Shizuoka Univ.*)  
 WADA, Takuro (*Shizuoka Univ.*)  
 YONETANI, Yoshiaki (*QST*)  
 MIYANISHI, Hisanori (*Nagoya Univ.*)  
 SAITO, Shinji (*IMS*)

Tritium is radioactive hydrogen and is mostly produced by nuclear reaction from human activity. Tritium decays to helium-3 by beta decay with emissions of a beta-ray and an antineutrino with a half-life of 12.323 years. Since the range

of beta rays emitted from tritium is short, external exposure is not problematic and protection against internal exposure is important. Beta rays may cause damage on macromolecules such as polymeric materials and DNA both directly and indirectly. Moreover, if substituted tritium in macromolecules decays to helium-3, their structure may be destabilized by chemical bond breakage, which is called decay effect. Although numerous experimental and computer simulation studies have been made on the damage of macromolecules through direct and indirect action, any studies have not been conducted on the damage of macromolecules through decay effect because of the difficulties in extracting the decay effect only.

In this project, we aim to predict the structural change of tritium-substituted macromolecules such as polymeric materials and DNA by a beta decay to helium-3 using molecular dynamics simulations.

Three meetings were held at IMS. Not only the core members (the applicants of this project) but also other related collaborators attended these meetings. The first two meetings were held to discuss the course of action for this project on June 6 and December 3, 2018. The third meeting was held to summarize the progress and discuss a future plan of this project on March 4–5, 2019.

### (b) Construction of Synthetic Microdomains to Artificially Assemble Biological Polymers on Lipid Membranes Using Metal Complex Lipids

OHTANI, Ryo (*Kyushu Univ.*)  
 KAWANO, Kenichi (*Kyoto Univ.*)  
 KINOSHITA, Masanao (*Kyushu Univ.*)  
 YANAKA, Saeko (*IMS*)  
 KATO, Koichi (*IMS*)

Cell membranes are nonuniform entities characterized by heterogeneous molecular assemblies that mediate biological processes exemplified by signal transduction. Accumulating evidence has indicated that these microdomains comprise various lipid molecules including glycosphingolipids and cholesterol and serve as molecular platforms where specific biomolecules accumulate to perform sophisticated functions. To gain a deeper understanding of these complex membrane functions, we employed a multilateral approach in an attempt to artificially control membrane properties and their molecular assembly.

In this project, we created and applied *metal complex lipids* for (1) manipulating lipid membrane properties such as curvature and viscosity to construct synthetic domain architectures and (2) controlling assemblies of biological polymers thereon. The metal complex lipid consists of a metal complex moiety as its hydrophilic head and an alkyl chain as its hydrophobic tail. It exhibits different physical properties from those of natural lipid species, which further impacts lipid membrane properties. Through investigation of the influence of the metal complex lipids on phase-transition and molecular-assembling behaviors of both artificial and cell membranes, we successfully constructed an artificial phase separation system with micro-sized metal complex domains in living cell membranes. We intend to observe the metal complex domains using high-speed atomic force microscopy. Moreover, synthesis of new metal complex lipids hybridizable to biomolecules is also underway.

## PROGRAMS

We held three collaboration meetings in the 2018 financial year to extensively discuss our research progress and future planning. The first and the third meetings were held at Yamate 3<sup>rd</sup> Blding 2F small meeting room on May 12, 2018, and

March 9, 2019, respectively. The second meeting was held at Kumamoto University on November 8, 2018, where RO was formerly posted.

### (2) Research Symposia

(From Oct. 2018 to Sep. 2019)

Dates	Theme	Chair
Oct. 28, 2018	The 1 <sup>st</sup> Hydride Ionics Seminar	<b>KOBAYASHI, Genki</b>
Nov. 30–Dec. 1, 2018	The International Symposium on Bioinorganic Chemistry 2018	<b>SHOJI, Osami</b> <b>AONO, Shigetoshi</b>
Jan. 15–16, 2019	Water at Interfaces 2018	<b>ONISHI, Hiroshi</b> <b>SUGIMOTO, Toshiki</b>
Mar. 3– 4, 2019	Coordination Chemistry for Controlling Hierarchical Structures and Functions	<b>UEMURA, Takashi</b> <b>MASAOKA, Shigeyuki</b>
Mar. 15–16, 2019	New Frontier in Protein Design & Engineering	<b>ARAI, Ryoichi</b> <b>KOGA, Nobuyasu</b>
May 21–22, 2019	Micro-Beam Analysis Workshop Atomic Level Imagings in Synchrotron-Radiation-Based Materials-Science Research	<b>MATSUI, Fumihiko</b>
May 28, 2019	The Challenge of Single Molecule Organic Chemistry	<b>NAKANISHI, Waka</b> <b>MOMIYAMA, Norie</b>
May 30, 2019	Fusion of Chemistry and Information Science —Toward New Innovative Chemistry—	<b>ADSCHIRI, Tadafumi</b> <b>YAMAMOTO, Hiroshi</b>
Jun. 10–11, 2019	Solid State Chemistry Forum	<b>KOBAYASHI, Genki</b>
Aug. 5– 6, 2019	Development of Novel Functional Molecular System Using Quantum Phase Degree of Freedom	<b>KAGAWA, Fumitaka</b> <b>YAMAMOTO, Hiroshi</b>
Aug. 8–10, 2019	Topological Physics and Organic Massless Dirac Systems	<b>TAJIMA, Naoya</b> <b>YOKOYAMA, Toshihiko</b> <b>NAKAMURA, Toshikazu</b>
Jun. 9, 2019	Meeting for Lectures at 59 <sup>th</sup> Summer School on Molecular Science for Young Scientists	<b>KOMATSUBARA, Wataru</b> <b>SUGIMOTO, Toshiki</b>
May 15–18, 2019	Chirality-Induced Spin Selectivity and Its Related Phenomena	<b>YAMAMOTO, Hiroshi</b>

**(3) Numbers of Joint Studies Programs**

Categories		Oct. 2018–Mar. 2019		Apr. 2019–Sep. 2019		Total		
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		2		1		3		3
Research Symposia		5		6		11		11
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		23	52	14	28	37	80	117
Use of Facility	Instrument Center		79		67		146	146
	Equipment Development Center	2	3	2	5	4	8	12
Use of UVSOR Facility		114	1	93	2	207	3	210
Use of Facility Program of the Computer Center						248*		248*

\* from April 2018 to March 2019