Special Research Projects

IMS has special research projects supported by national funds. Three projects in progress are:
(a) MEXT Nanotechnology Platform Program
Platform of Molecule and Material Synthesis
(b) Inter-University Network for Efficient Utilization of Research Equipments
(c) MEXT Program Advanced Research Infrastructure for Materials and Nanotechnology in Japan:
Spoke Organization in Advanced Material Circulation Techniques

These three projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(a) MEXT Nanotechnology Platform Program Platform of Molecule and Material Synthesis

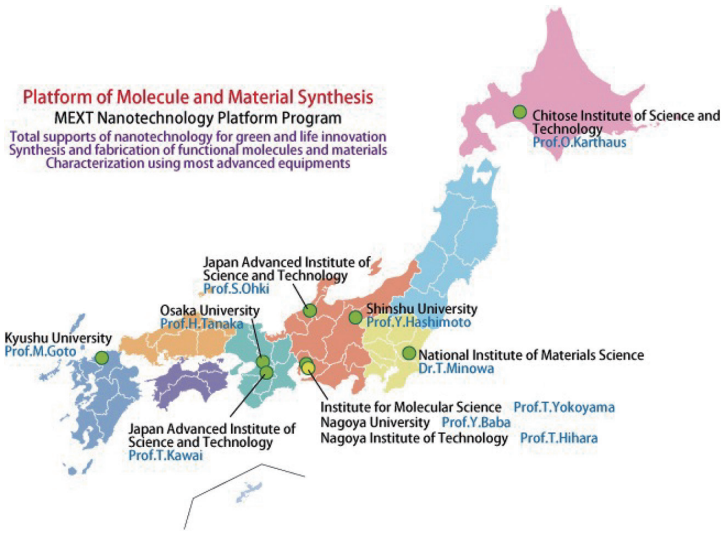
Since July 2012, Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT) has been conducted in order to promote public usage of various nanotechnology facilities. This program will continue until March 2022 and consists of three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the management center of the platforms. Each platform consists of about ten organizations all over Japan. IMS conducts a representative core organization of the Molecule and Material Synthesis Platform. All the organizations in this platform are shown in Figure. In this platform, to promote green and life innovation researches using nanotechnology related techniques not only for universities and government institutes but also for private companies, we will open various kinds of our facilities with total supports including molecular synthesis, materials fabrications, characterization, data analysis and scientific discussion. We will encourage applications not only to each element, but to combined usage of several supporting elements for biotechnology and green chemistry. In IMS, the number of accepted proposals in FY2020 amounted 128 (111 non-proprietary and 10 proprietary proposals, excluding inhouse applications from IMS) and the total number of days used for the supports is 2127 (1960 days for non-proprietary proposals and 50 days for proprietary ones).

List of Supports in IMS (FY2020)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, Y. Toyama
Organization Management in IMS			Y. Hyodo, Y. Funaki
UVSOR Synchrotron Radiation	X-Ray Magnetic Circular Dichroism	T. Yokoyama	T. Koitaya, K. Yamamoto, O. Ishiyama
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Aoyama, T. Kondo, N. Takada, S. Kimura, T. Kikuchi, N. Mizutani, A. Ishikawa
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Aoyama, T. Kondo, T. Toyota, J. Mathuo
Electron Microscopy	Field Emission Scanning Electron Microscopy	T. Yokoyama	O. Ishiyama, A. Toyama
	Low Vacuum Analytical Scanning Electron Microscopy		
	Field Emission Transmission Electron Microscope		S. Iki, T. Ueda, M. Uruichi
X-rays	Single Crystal X-Ray Diffractometer		Y. Okano
	Low Temperature Single Crystal X-Ray Diffractometer for Microcrystals		
	Molecular Structure Analysis using Crystalline Sponge Method		M. Fujita, T. Mitsuhashi
	Powder X-Ray Diffractometer		M. Fujiwara
	Operando Multi-Purpose X-Ray Diffraction		G. Kobayashi, F. Takeiri, M. Fujiwara
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama
Electron Spectroscopy	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	S. Kera, K. Tanaka	S. Ideta

PROGRAMS

Electron Spin Resonance	Pulsed High Field ESR	T. Yokoyama, T. Nakamura	M. Asada, M. Fujiwara, S. Iki, T. Ueda
	X-Band CW ESR		
	X, Q-Band CW ESR		
SQUID	Superconducting Quantum Interference Device		M. Asada, M. Fujiwara, S. Iki
Thermal Analysis	Differential Scanning Calorimeter (Solutions)	T. Yokoyama	T. Mizukawa, M. Uruichi, H. Nagao
	Isothermal Titration Calorimeter (Solutions)		
	Calorimeter for solids		M. Fujiwara
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		T. Mizukawa, M. Uruichi, K. Fujikawa
Spectroscopy	Microscopic Raman Spectroscopy		M. Uruichi
	Fourier Transform Far Infrared Spectroscopy		
	Fluorescence Spectroscopy		T. Ueda
	Ultraviolet & Visible Absorption Spectroscopy		
	Circular Dichroism		T. Mizukawa, M. Uruichi, K. Fujikawa
Lasers	Picosecond Laser		T. Ueda
High Field NMR	800 MHz Solutions, Cryostat Probe	K. Kato	M. Yagi, S. Yanaka, Y. Isono
	600 MHz Solids	K. Nishimura	
	600 MHz Solutions	T. Yokoyama	T. Mizukawa, M. Uruichi, H. Nagao
Functional Molecular Synthesis and Molecular Device Fabrication	Organic Thin Film Solar Cells	M. Hiramoto	S. Izawa
	Organic Field Effect Transistors	H. Yamamoto	D. Hirobe
	Functional Organic Synthesis	N. Momiyama, T. Suzuki	N. Ohtsuka, T. Fujinami
	Large Scale Quantum Mechanical Calculations	M. Ehara	
	Magnetic Thin Films	T. Yokoyama	T. Koitaya, K.Yamamoto
	Metal Complexes	T. Kusamoto	R. Matsuoka
	Inorganic Materials	G. Kobayashi	F. Takeiri
	Biomolecule System	S. Akiyama	A. Mukaiyama, Y. Furuike
	Supplementary Apparatus in Instrument Center	T. Yokoyama	



(b) Inter-University Network for Common Utilization of Research Equipments

It is highly important to improve instrumental supporting environments for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting researches and educations with high standard quality. To install such sophisticated instruments, tremendous amount of budgets would be necessary. In 2007, for constructing a national-wide network to provide easy accesses to high-level equipments to researchers and students in universities all over Japan, the five-year project "Functioning of Inter-University Network for Efficient Utilization of Chemical Research Equipments" was launched. The network maintains an internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. 72 national universities as well as Institute for Molecular Science (total 73 organizations) all over Japan have been participating in the network. They are grouped into 12 local regions and in each region the regional committee discusses and determines the operation of regional network systems with the hub university chairing. There is no barrier for every user to access to any universities beyond his/her regional group. From 2009, the registered equipments are open to the researchers and students of all the public (prefectural *etc.*) and private universities. Since 2010, the project has been renamed "Inter-University Network for Common Utilization of Research Equipments" still keeping the original strategy and stable functioning. Since 2018, the institutions that provide research facilities are open to public and private universities. Currently, the network is organized by 78 organizations. The number of registered users amounts to 15,000 in 500 universities/institutions/companies covering over 4,000 laboratories in Japan (July, 2021). Network usage reaches about 150,000 times a year, and the number continues to grow. Moreover, we have actively provided various opportunities where technical staffs and users can improve their technical skills and frankly communicate with each other.

(c) MEXT Program Advanced Research Infrastructure for Materials and Nanotechnology in Japan: Spoke Organization in Advanced Material Circulation Techniques

In fiscal year of 2021, "Advanced Research Infrastructure for Materials and Nanotechnology in Japan" program supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT) just started, succeeding to MEXT Nanotechnology Platform program that will be finished in 2021. In this new program, six Hub&Spoke teams are constructed with the Center Hub of National Institute of Materials Science (NIMS), and IMS belongs to the Hub&Spoke team of Advanced Material Circulation Techniques with NIMS (Hub), Nagoya Institute of Technology (Spoke), and The University of Electro-Communications (Spoke). Domestic and international equipment sharing is a most important purpose in this program as in the Nanotechnology Platform program. Moreover, users and staffs are requested to provide experimentally obtained data to the Data Platform that are being constructed in NIMS. The accumulated data will be open to all researchers for future material scientific investigations. Human resource development is also an important aim in this program. In IMS, this program is mainly managed by Instrument Center, supported by Research Center for Computational Science in data storage and transfer to NIMS Data Platform. Although practical executions start from next fiscal year, similar equipment sharing will be conducted as in the Nanotechnology Platform program. In 2021, a new electron spin resonance system will be installed through the program. We hope that this program will successfully be performed and equipment sharing usage in IMS will further be accelerated.

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) 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.

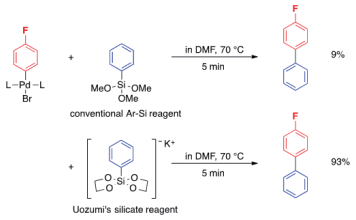
In this project, we created and applied *metal complex lipids* for (1) manipulating lipid membrane properties such as curvature and viscosity to construct synthetic domain architectures and (2) controlling assemblies of biological polymers thereon. The metal complex lipid consists of a metal complex 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 rigid domains consisting of metal complexes in living cell membranes. Furthermore, we succeeded in synthesizing a new metal complex lipid which could provide unique fluid–fluid phase separation in lipid membranes. The metal complex lipid not only exhibits such domain formation property but also offers a possibility to hybridize with biomolecules via the click chemistry approach due the head part incorporating an ethynyl substituent. We expect that this metal complex lipid will be applicable to assembling and accumulating biomolecules in lipid membranes, which is now underway.

We held a collaboration meeting in 2020 to extensively discuss our research progress and future planning. The meeting was held at on-line on July 29th, 2020. This project has achieved two published papers (R. Ohtani *et al. Angew. Chem., Int. Ed.* **61**, 13603–13608 (2021), R. Ohtani *et al. Angew. Chem., Int. Ed.* **59**, 17931–17937 (2020)).

(b) *Operando* Structural Studies on the Reacting Species of the Cross-Coupling Catalysis

FUJIKAWA, Shigenori (*Kyushu Univ.*)
TAKAYA, Hikaru (*Kyoto Univ. and IMS (cross appointment)*)
NAGASAKA, Masanari (*IMS*)
OKUMURA, Shintaro (*IMS*)
UOZUMI, Yasuhiro (*IMS*)

The palladium-catalyzed cross-coupling reactions have been recognized as the most powerful synthetic means of carbon–carbon bond formation. Coupling of aryl halides and organosilicon reagents, the so-called Hiyama coupling, is one of the representatives. Recently, Uozumi at IMS developed aryl silicate reagents which exhibited remarkably high reactivity toward the Hiyama coupling with aryl halides (Scheme 1). These observations prompted us to examine the operando structural studies on the aryl silicates as well as conventional aryl silyl reagents under the actual coupling reaction conditions by *in situ* NEXAFS measurements. For the preliminary measurements, the electronic structures of phenyl groups in



Scheme 1. The Hiyama Coupling Reactions with Uozumi's Aryl Silicate.

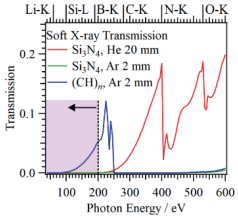


Figure 1. Calculated soft X-ray transmission at several conditions of liquid cells.

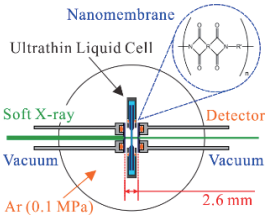


Figure 2. The schematic of an ultrathin liquid cell including Si-free nanomembranes.

organosilicon compounds were investigated by C K-edge NEXAFS (280 eV) at BL3U of UVSOR-III (by Nagasaka, Okumura). From the soft X-ray transmission calculations (Figure 1), on the other hand, the Si L-edge NEXAFS (100 eV) needs the ~2 mm optical length of argon gas and Si-free nanomembranes. Thus, this project combines (1) a new coupling reaction (by Uozumi, Okumura) and (2) an ultrathin liquid cell that achieves the 2.6 mm optical length of argon gas (by Nagasaka, Takaya) including novel Si-free nanomembranes developed by Fujikawa at Kyusyu University (Figure 2) at once to realize the *operando* structural studies of the highly reactive Hiyama coupling reaction. Though, in 2021, this project team have never had the on-site collaborations because of the COVID catastrophe, we have prepared the reacting reagents, Si-free nanomembranes, and an ultrathin liquid NEXAFS cell at each site. This *in situ* NEXAFS method will pave the way for studying various organic reaction with organosilicon, organolithiums, organoboranes, and so on.

(2) Research Symposia

(From Oct. 2020 to Sep. 2021)

Dates	Theme	Chair
Oct. 28–29, 2020	Next Generation Spectro-Mircroscopy and Micro-Spetroscopy Workshop	**OHIGASHI, Takuji**
Dec. 4– 5, 2020	New Development of Molecular Manipulation and Reaction Control Interwoven by Nanospace and Light	**MINAMIMOTO, Hiro** **OKAMOTO, Hiromi**
Mar. 11–12, 2021	The Potential for Academic Development Originating in Coordination Chemistry	**MATSUDA, Ryotaro** **KUSAMOTO, Tetsuro**
Jul. 12–13, 2021	IMS-FHI Symposium “Emerging Techniques of Scanning Probe Microscopy”	**KUMAGAI, Takashi**
Aug. 31, 2021	The Morino Discussion 2021	**MUNAKATA, Toshiaki** **SUGIMOTO, Toshiki**
Aug. 16–19, 2021	The 60th Summer School of Molecular Science by Young Scientistse	**TOKITA, Tsukasa** **SUGIMOTO, Toshiki**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2020–Mar. 2021		Apr. 2021–Sep. 2021			Total			
		Regular	NanoPlat	Regular	NanoPlat	NMRPlat	Regular	NanoPlat	NMRPlat	Sum
Special Projects		1		1			2			2
Research Symposia		3		2			5			5
Research Symposia for Young Researchers		0		2			2			2
Cooperative Research		30	27	20	30	3	50	57	3	110
Use of Facility	Instrument Center		74		69		0	143		143
	Equipment Development Center	1	5	0	5		1	10		11
Use of UVSOR Facility		15	1	101	1		116	2		118
Use of Facility Program of the Computer Center							271*			271*

* from April 2020 to March 2021

Collaboration Programs

(1) MOU Partnership Institutions

IMS has concluded academic exchange agreements with overseas institutions.

The agreements encourage

- Exchange of researchers
- Internship of students and postdoctoral fellows
- Joint research workshops
- Joint research laboratories

Institution	Period	Accept*	Send*
The Korean Chemical Society, Physical Chemistry Division [Korea]	2006.12–2022.10	0	0
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2005. 1–2023. 1	0	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2009.10–2024.10	0	0
Freie Universität Berlin (FUB) [Germany]	2013. 6–2022. 6	0	0
National Nanotechnology Center, National Science and Technology Development Agency (NANOTEC/NSTDA) [Thailand]	2017.10–2022.10	0	0
Sungkyunkwan University, Department of Chemistry (SKKU) [Korea]	2018. 4–2022. 3	0	0
University of Oulu [Finland]	2021. 5–2024. 5	0	0
National Yang Ming Chiao Tung University [Taiwan]	2018. 6–2023. 5	0	0
Peter Grünberg Institute, Forschungszentrum Jülich GmbH (FZJ) [Germany]	2018.10–2023. 9	0	0
State Key Laboratory of Physical Chemistry of Solid Surfaces (Xiamen University) [China]	2019.12–2024.12	0	0
Indian Institute of Technology Kanpur [India]	2020. 4–2025. 3	0	0
Fritz-Haber-Institut der Max-Planck-Gesellschaft [Germany]	2021. 4–2023. 3	0	1

* No. of researchers during the period from Sep. 2020 to Aug. 2021

Academic Exchange Agreement with Overseas Universities/Institutes (SOKENDAI) as follows ;

Institution	Period	Accept*	Send*
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2021. 4	0	0
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2024.11	0	0
Vidyasirimedhi Institute of Science and Technology [Thailand]	2018. 9–2023. 9	3	0
Friedrich Schiller University Jena [Germany]	2020. 7–2023. 7	0	0

* No. of researchers during the period from Sep. 2020 to Aug. 2021

(2) International and Inter-Institutional Collaboration Symposia

Several international symposia and workshops in molecular science are held in IMS and in Japan. Some workshops are organized with our MOU partners for international collaboration in the MOU partner's country as well as in Japan:

Program	Coordinator	Date	Place
Next Generation Spectro-Microscopy and Micro-Spectroscopy Workshop	MATSUI, Fumihiko (IMS) OHIGASHI, Takuji (IMS)	2020.10.28–29	Online
1st IMS-FHI Symposium "Emerging Techniques of Scanning Probe Microscopy"	KUMAGAI, Takashi (IMS)	2021.7.21	Online

(3) IMS International Internship Program

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	3*	–

* from Sep. 2020 to Aug. 2021

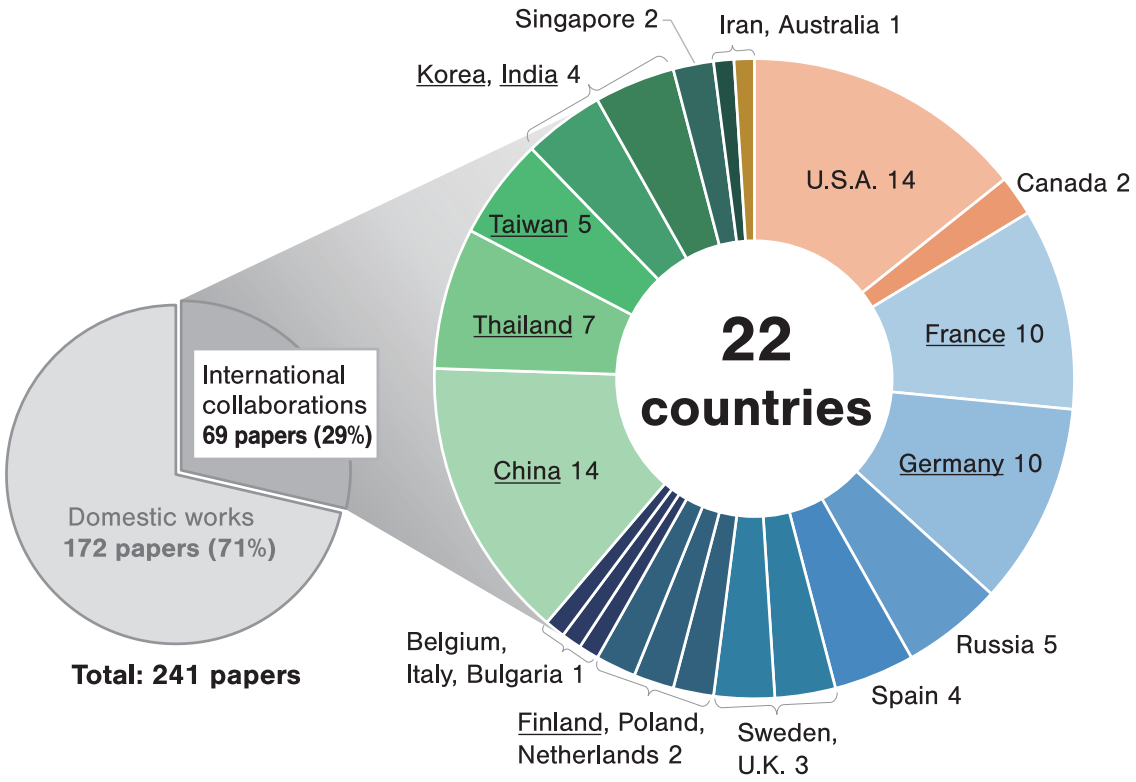
(4) IMS International Collaboration (Including online meetings)

Category	Number of People
International Joint Research Programs	79
International Use of Facilities Programs	14

from Sep. 2020 to Aug. 2021

Internationally Collaborated Publications

Articles and reviews published in 2020



Underlined countries include MOU Partnership Institutions
Scopus dataset, Nov. 2021