Special Research Projects

IMS has special research projects supported by national funds. Four projects in progress are:

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

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

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

(d) MEXT Project for Promoting Public Utilization of Advanced Research Infrastructure (support for formation of advanced research platforms): NMR PLATFORM

These four 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.

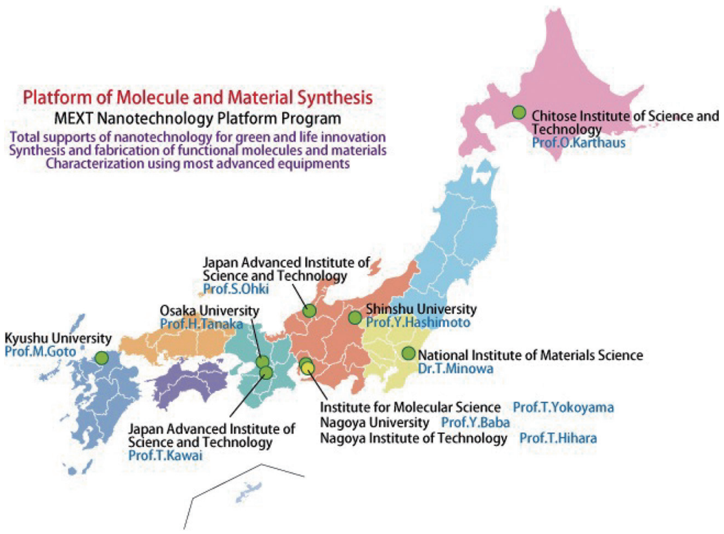
(a) MEXT Nanotechnology Platform Program Platform of Molecule and Material Synthesis

Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT) was conducted from July 2012 to March 2022 in order to promote public usage of various nanotechnology facilities. This program consisted of three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the management center of the platforms. About ten organizations from all over Japan took part in each platform. IMS conducted 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 opened various kinds of our facilities with total supports including molecular synthesis, materials fabrications, characterization, data analysis and scientific discussion. We encouraged 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 FY2021 amounted 125 (116 non-proprietary and 9 proprietary proposals, excluding inhouse applications from IMS) and the total number of days used for the supports is 2,969 (2,720 days for non-proprietary proposals and 38 days for proprietary ones).

List of Supports in IMS (FY2021)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, K. Nakamoto
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	T. Kondo, N. Takada, S. Kimura, T. Kikuchi, N. Mizutani, A. Ishikawa
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		T. Kondo, T. Toyota, J. Mathuo
Electron Microscopy	Field Emission Scanning Electron Microscopy	T. Yokoyama	O. Ishiyama, A. Toyama, T. Ueda
	Low Vacuum Analytical Scanning Electron Microscopy		
	Field Emission Transmission Electron Microscope		S. Iki, T. Ueda, M. Uruichi
Scanning Probe Microscope	Scanning Probe Microscope		T. Minato, T. Ueda, T. Sugimoto
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, M. Miyajima
	Operando Multi-Purpose X-Ray Diffraction		G. Kobayashi, F. Takeiri, M. Fujiwara, M. Miyajima
	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	
	X-Ray Photoelectron Spectroscopy	T. Yokoyama	T. Koitaya, K. Yamamoto, O. Ishiyama
Electron Spin Resonance	Pulsed High Field ESR	T. Yokoyama, T. Nakamura	M. Asada, M. Fujiwara, S. Iki, T. Ueda, M. Miyajima
	X-Band CW ESR		
	X, Q-Band CW ESR		
SQUID	Superconducting Quantum Interference Device		M. Asada, M. Fujiwara, S. Iki, M. Miyajima
Thermal Analysis	Differential Scanning Calorimeter (Solutions)	T. Yokoyama	M. Uruichi, H. Nagao
	Isothermal Titration Calorimeter (Solutions)		
	Calorimeter for solids		M. Fujiwara, M. Miyajima
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		M. Uruichi, K. Fujikawa
Spectroscopy	Microscopic Raman Spectroscopy		M. Uruichi
	Fourier Transform Far Infrared Spectroscopy		
	Fluorescence Spectroscopy		T. Ueda
	Ultraviolet & Visible Absorption Spectroscopy		
	Absolute PL Quantum Yield Measurement		
	Circular Dichroism		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	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, T. Sato
	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. From 2009, the registered equipments are open to the researchers and students of all the public (prefectural *etc.*) and private universities and private companies. 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 16,000 in 550 universities/institutions/companies covering over 4,300 laboratories in Japan (July, 2022). Network usage reaches about 170,000 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

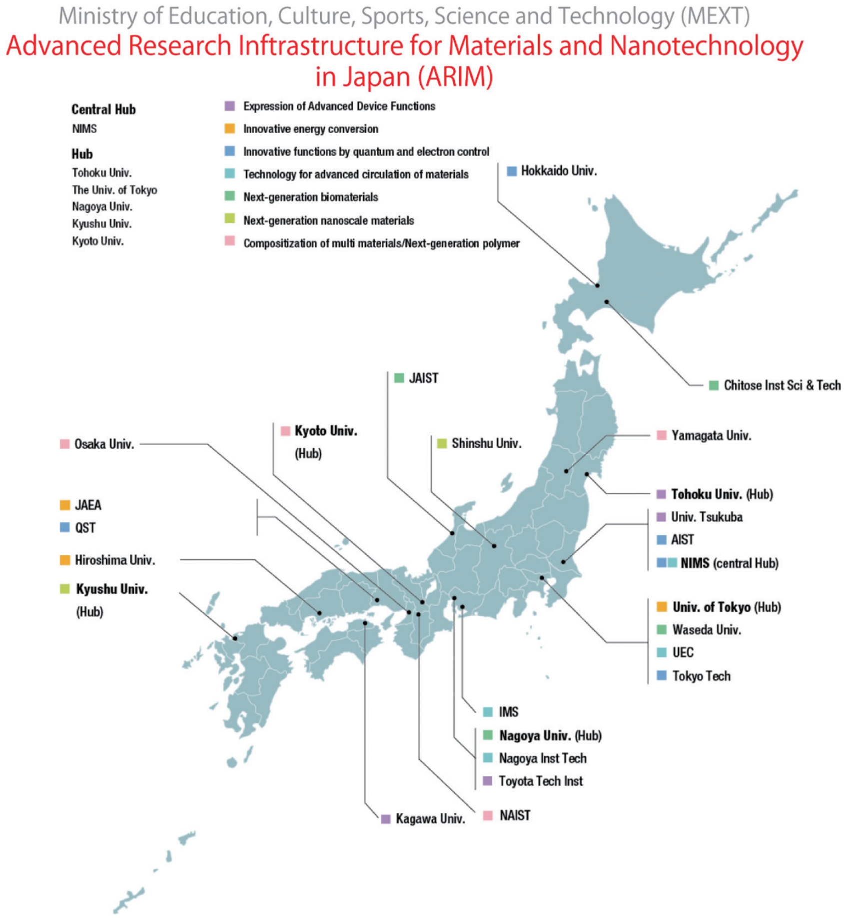
Since 2021, ARIM (Advanced Research Infrastructure for Materials and Nanotechnology in Japan) program supported by MEXT (Ministry of Education, Culture, Sports, Science and Technology) has been conducted, succeeding to MEXT Nanotechnology Platform program that was completed in March, 2022. In this new program, seven "key technology domains" are set. Each key technology domain team consist of one hub organization and several spoke organizations, with the center hub of National Institute of Materials Science (NIMS). The hub & spoke networks for collecting, accumulating, and structuring research data that are created from observation, measurement, synthesis and fabrication equipment and facilities, were launched in order to strengthen AI-driven materials & device R&D using informatics techniques. IMS belongs to one of the key technology domains of "Technology for advanced circulation of materials" lead by the NIMS hub, together with the spoke organizations of Nagoya Institute of Technology and The University of Electro-Communications. Domestic and international equipment sharing is the 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 Center (DPC) that are being constructed in NIMS. Accumulated structured data will be shared through the NIMS DPC. In addition, we will contribute to strengthening material innovation force by building a "Material DX Platform" in collaboration with the Materials Data Creation and Utilization R&D Project. In this program, three areas of shared methodology are set to promote cooperation across the seven key technology domains. IMS also acts as a representative organization for the cross-sectional technological area concerning the material synthesis process to promote technological cooperation among all the participating organizations. Human resource development is also an important aim in this program and IMS regularly conducts training sessions with "EQ-NET" to upskilling of the technical staffs engaged in this program. In IMS, the mission for the ARIM program is mainly organized by Instrument Center, supported by Research Center for Computational Science in data storage and transfer to NIMS DPC. Because in 2021 equipment sharing was conducted through the Nanotechnology Platform program, this year FY2022 is the first year in this program, and equipment sharing is being conducted as previously, while the data accumulation mission is progressively in preparation. Through this program, a new electron spin resonance (ESR) system was installed in IMS last year, and also a new superconducting quantum interference device (SQUID) magnetometer will be introduced at the end of FY2022. We hope that this program will successfully be performed and equipment sharing and data sharing will be accelerated.

List of Equipment Supports in IMS Spoke (FY2022)

Supporting Element	Responsible Persons	Charging Persons
Organization Management in IMS Spoke	T. Yokoyama	T. Nakamura, M. Ehara, K. Iwahashi, T. Suzuki, K. Nakamoto, Y. Ota, M. Kaku, Y. Funaki, Y. Hyodo
Organization Management in Cross-Sectional Technological Area of Material Synthesis	T. Yokoyama	Y. Ota, K. Nakamoto, M. Kaku, Y. Kurita, A. Ishikawa

PROGRAMS

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	T. Kondo, T. Kikuchi, S. Kimura, N. Takada, A. Ishikawa
	3D Optical Surface Profiler		
	Electron Beam Lithgraphy		
Electron Microscopy	Field Emission Scanning Electron Microscopy	T. Yokoyama	O. Ishiyama
	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		
	Powder X-Ray Diffractometer		M. Fujiwara, M. Miyajima
	Operando Multi-Purpose X-Ray Diffraction		G. Kobayashi, F. Takeiri, M. Fujiwara, M. Miyajima
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama, Y. Furuike
	Molecular Structure Analysis using Crystalline Sponge Method	M. Fujita	T. Mitsuhashi, T. Yokoyama
Electron Spectroscopy	X-Ray Photoelectron Spectroscopy	T. Yokoyama	T. Koitaya, S. Iki, K. Yamamoto, O. Ishiyama
	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	S. Kera, K. Tanaka	K. Fukutani
Electron Spin Resonance	Pulsed High Field ESR	T. Yokoyama, T. Nakamura	M. Asada, M. Fujiwara, M. Miyajima, S. Iki, T. Ueda
	X-Band CW ESR		
	X, Q-Band CW ESR		
	Pulsed ESR		
SQUID	Superconducting Quantum Interference Device		M. Asada, M. Fujiwara, M. Miyajima, S. Iki
Thermal Analysis	Differential Scanning Calorimeter (Solutions)	T. Yokoyama	H. Nagao, M. Uruichi
	Isothermal Titration Calorimeter (Solutions)		
	Calorimeter for solids		M. Fujiwara, M. Miyajima
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		M. Uruichi, K. Fujikawa
Spectroscopy	Microscopic Raman Spectroscopy		M. Uruichi, K. Fujikawa
	Fourier Transform Far Infrared Spectroscopy		
	Fluorescence Spectroscopy		T. Ueda
	Ultraviolet & Visible Absorption Spectroscopy		
	Absolute Photoluminescence Quantum Yield Spectrometer		
	Circular Dichroism		T. Mizukawa, M. Uruichi, K. Fujikawa
Lasers	Picosecond Laser		T. Ueda
High Field NMR	600 MHz Solids	K. Nishimura	
	600 MHz Solutions	T. Yokoyama	T. Mizukawa, M. Uruichi, H. Nagao
Functional Molecular Synthesis and Molecular Device Fabrication	Organic Field Effect Transistors	H. Yamamoto	T. Sato
	Organic Synthesis DX	T. Suzuki	N. Momiyama, N. Ohtsuka
	Large Scale Quantum Mechanical Calculations	M. Ehara	Y. Kanazawa
	Magnetic Thin Films	T. Yokoyama	T. Koitaya, K.Yamamoto
	Metal Complexes	T. Kusamoto	R. Matsuoka
	Supplementary Apparatus in Instrument Center	T. Yokoyama	



(d) MEXT Project for Promoting Public Utilization of Advanced Research Infrastructure (support for formation of advanced research platforms): NMR PLATFORM

MEXT has been working on "Project for Promoting Public Utilization of Advanced Research Infrastructure (support for formation of advanced research platforms)" to maintain and advance the world's leading R&D infrastructure by forming platforms for shared use to construct a network of research facilities/equipment. The objective is to contribute to the sustainable maintenance and improvement of R&D infrastructures in Japan by forming a nationwide advanced research platforms for all researchers.

In this context, the NMR PLATFORM is based on a network of advanced NMR facilities that can be shared by industry, academia, and government. Under this platform, research institutions that have cutting-edge NMR research facilities and knowledge work closely to provide opportunities for researchers from diverse disciplines and organizations around the nation to use their facilities. Furthermore, the objective is to establish a system that contributes to the promotion of R&D and the creation of innovation throughout Japan. The NMR PLATFORM is conducted by RIKEN, the representative organization, eight universities or research institutes, all of which have established an advanced NMR research infrastructure, and four manufacturers of related NMR technologies and products.

IMS began participating in NMR PLATFORM in FY2021, aiming to enhance overall scientific and technological activities by providing an 800-MHz solution NMR spectrometer for a wide range of uses in industry and academia. In addition, the project is developing initiatives to support researchers in various fields at universities and research institutes through the shared use of NMR equipment. ExCELLS has been participating in this project on behalf of IMS since FY2022.

Joint Studies Programs

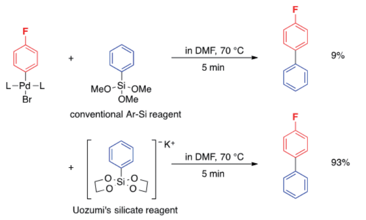
As one of the important functions of an inter-university research institute, IMS facilitates joint studies programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and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

(1) Special Projects

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

FUJIKAWA, Shigenori (*Kyushu Univ.*)
TAKAYA, Hikaru (*Teikyo Univ. Sci. and IMS (concurrent)*)
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 the joint project that examines 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. Figure 1 shows the carbon K-edge NEXAFS spectrum of 100 mM trimethoxy(phenyl)silane (Ph-Si(OMe)$_3$) in tetrahydrofuran (THF) measured at BL3U of UVSOR-III Synchrotron (by Okumura, Nagasaka, Uozumi). The C=C π* peak of phenyl groups in Ph-Si(OMe)$_3$ is observed even in organic solvent containing carbon atoms since the peaks of THF exist at the higher energy side. We have investigated the C–Si bond length of several organosilicon compounds by C K-edge NEXAFS experiments and inner-shell quantum chemical calculations and have discussed the relation of the reaction mechanism of Hiyama coupling reaction. This project also aims to achieve the Si L-edge NEXAFS measurements of organosilicon compounds under the actual reaction conditions by the combination of (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 (Figure 2). In the present status, we have tested the ultrathin liquid cell including Si-free nanomembranes by using a conventional FT-IR system (by Nagasaka) and will apply the Si L-edge NEXAFS measurements at BL3U of UVSOR-III in this year.



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

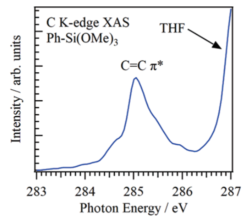


Figure 1. C K-edge NEXAFS spectrum of 100 mM Ph-Si(OMe)$_3$ in THF.

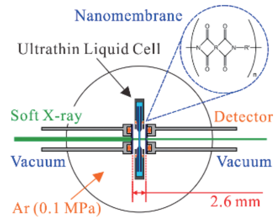


Figure 2. The schematic of an ultrathin liquid cell including Si-free nanomembranes.

(b) Analysis and Elucidation of Deactivation Mechanism for High Durability of Metal Complex-Carbon Electrodes for Electroreduction of CO_2 in Water

SAITO, Susumu (*Nagoya Univ.*)
SATO, Shyunsuke (*Toyota Central R&D Labs., Inc.*)
SUGIMOTO, Toshiki (*IMS*)

In order to investigate the cause of the performance degradation of the cathode electrode during the ongoing electroreduction of CO_2 in water using a complex-carbon electrode,[1] *in-situ* observations of the cathode electrode are performed using third-order nonlinear vibrational spectroscopy. We have jointly constructed an electrolysis cell for spectroscopy equipped with an anhydrous quartz window, which is the most suitable material for measurement. Using this spectroscopic cell, we first optimized the optical system for third-order nonlinear spectroscopic measurement for the complex-carbon electrode installed in the reaction cell. As the next step, we are going to conduct third-order nonlinear vibrational spectroscopy to identify the cause of the deterioration of the electrode performance, while systematically changing the reaction conditions such as the temperature, pH, applied voltage, and CO_2 concentration of the aqueous solution.

Reference

1) M. Yamauchi, H. Saito, T. Sugimoto, S. Mori and S. Saito, *Coord. Chem. Rev.* **472**, 214773 (2022).

(2) Research Symposia

(From Oct. 2021 to Sep. 2022)

Dates	Theme	Chair
Feb. 28–Mar. 1, 2022	Current Status and Future Prospects for Attosecond Laser Facility (ALFA)	**YAMANOUCHI, Kaoru** **OKAMOTO, Hiromi**
Mar. 8, 2022	Frontiers in Energy Science: Towards Cross-Hierarchical Understanding	**NAKAMURA, Toshikazu** **YAMAMOTO, Hiroshi**
Sep. 7, 9, Nov. 8–17, 2021	Study of Spin Transport Unique to Chiral Materials	**SUZUKI, Yuta** **YAMAMOTO, Hiroshi**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2021–Mar. 2022			Apr. 2022–Sep. 2022		Total			
		Regular	NanoPlat	NMRPlat	Regular	ARIM	Regular	NanoPlat/ ARIM	NMRPlat	Sum
Special Projects		1			1		2			2
Research Symposia		2			3		5			5
Research Symposia for Young Researchers		0			1		1			1
Cooperative Research		27	36	1	22	14	49	50	1	100
Use of Facility	Instrument Center		78			59		137		137
Use of Facility	Equipment Development Center	0	4		0	4	0	8		8
Use of Facility	UVSOR	110	2		103	2	213	4		217
Use of Facility Program of the Computer Center							278*			278*

* from April 2021 to March 2022

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]	2006.12–2026.10	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	7	1
Freie Universität Berlin (FUB) [Germany]	2013. 6–2025. 6	1	0
National Nanotechnology Center, National Science and Technology Development Agency (NANOTEC/NSTDA) [Thailand]	2017.10–2027.10	0	1
Sungkyunkwan University, Department of Chemistry (SKKU) [Korea]	2018. 4–2026. 3	0	0
University of Oulu [Finland]	2021. 5–2024. 5	2	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	1	0
Fritz-Haber-Institut der Max-Planck-Gesellschaft [Germany]	2021. 4–2023. 3	0	2

* No. of researchers during the period from Oct. 2021 to Sep. 2022

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

Institution	Period	Accept*	Send*
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2026. 3	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	1	1
Friedrich Schiller University Jena [Germany]	2020. 7–2023. 7	1	0
Chulalongkon University [Thailand]	2010. 4–2027. 9	0	1

* No. of researchers during the period from Oct. 2021 to Sep. 2022

(2) IMS International Internship Program

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	13*	–

* from Oct. 2021 to Sep. 2022

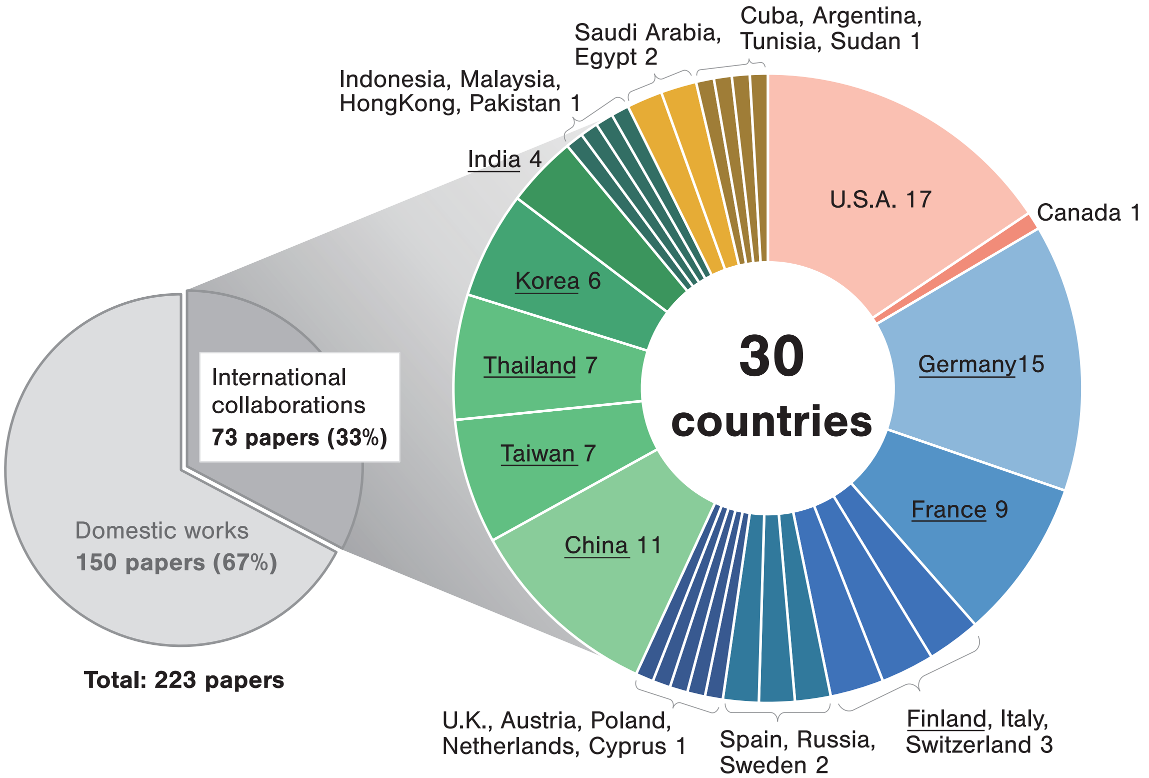
(3) IMS International Collaboration (Including online meetings)

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

from Oct. 2021 to Sep. 2022

Internationally Collaborated Publications

Articles and reviews published in 2021



Underlined countries include MOU Partnership Institutions
Scopus dataset, Oct. 2022