Special Research Projects

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

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

(b) MEXT Program Advanced Research Infrastructure for Materials and Nanotechnology in Japan: Spoke Organization in Advanced Materials Recycling Technologies and Representative Organization in Cross Sectional Technical Domain of Materials Synthesis Process

(c) "Development of Cold-Atom Based Quantum Simulators and Their Applications to Quantum Computing" within the Framework of Japan's Flagship Program on Quantum Sciences and Technologies "Q-LEAP" by MEXT and "PRISM" by the Cabinet Office of Japan (2018–2028)

(d) "Large-Scale and High-Coherence Fault-Tolerant Quantum Computer with Dynamical Atom Arrays" Supported by the Cabinet Office/JST Program "Moonshot Goal 6": Realization of a Fault-Tolerant Universal Quantum Computer That Will Revolutionize Economy, Industry, and Security by 2050

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.

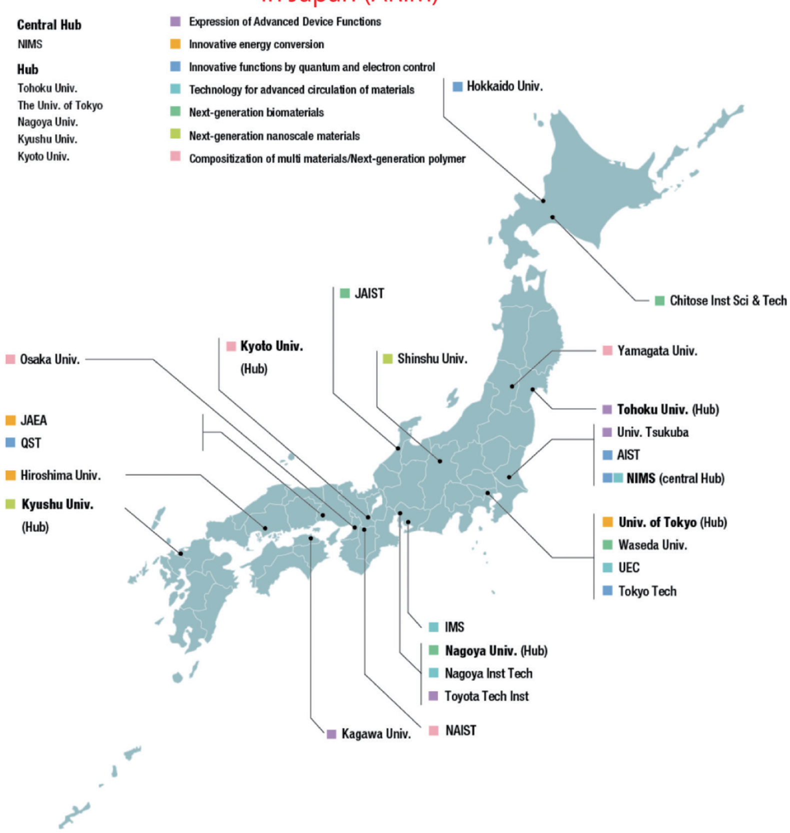
(a) Inter-University Network for Common Utilization of Research Equipments

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 17,000 in ~600 universities/institutions/companies (as of March, 2023). Network usage reaches more than 170,000 times a year, in which external usage amounts to 3,800 times, and these numbers continue 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.

(b) MEXT Program Advanced Research Infrastructure for Materials and Nanotechnology in Japan: Spoke Organization in Advanced Materials Recycling Technologies and Representative Organization in Cross Sectional Technical Domain of Materials Synthesis Process

Since 2021, ARIM (Advanced Research Infrstructure for Materials and Nanotechnology in Japan) program supported by MEXT (Ministry of Education, Cultre, Sports, Science and Technology) has been conducted, succeeding to MEXT Nanotechnology Platform progrm that was completed in March, 2022. In this new program, seven "key technology domains" are set. Each key technlogy domain team consist of one hub organization and several spoke organizations, with the center hub of NationalInstitute of Materials Science (NIMS). The hub & spoke networks for collecting, accumulating, and structuring reseach data that are created from observation, measurement, synthesis and fabrication equipment and facilities, were launhed in order to strengthen AI-driven materials & device R&D using informatics techniques. IMS belongs to one ofthe key technology domains of "Advanced materials recycling technologies" led by the NIMS hub, together with the spoke organizations of Nagoya Institute of Technology and The University of Electro-Communications. Domesic and international equipment sharing is the most important purpose in this program, as in the Nanotechnology Plaform program. Moreover, users and staffs are requested to provide experimentally obtained data to the Data Platfor Center (DPC) that are being constructed in NIMS. Accumulated structured data will be shared through the NIS DPC. In addition, we will contribute to strengthening material innovation force by building a "Material D Platform" in collaboration with the Data creation/utilization type material research and development project. In ths program, three areas of shared methodology are set to promote cooperation across the seven key technology domins. IMS also acts as a representative organization for the cross-sectional technological area concerning the maerial synthesis process to promote technological cooperation among all the participating organizations. Human resouce development is also an important aim in this program and IMS regularly conducts training sessions with “EQ-NT” to upskilling of the technical staffs engaged in this program. In IMS, the mission for the ARIM program is mainly rganized by Instrument Center, supported by Research Center for Computational Science in data storage and transfer t NIMS DPC. Because in 2021 equipment sharing was conducted through the Nanotechnology Platform program, FY2022 is the first year for equipment sharing in this program, while the data accumulation mission is in pogress. Through this program, a new electron spin resonance (ESR) system and a new superconducting quantum inteference device (SQUID) magnetometer were installed in IMS in 2021 and 2022, and a high-throughput low-temperatur single-crystal x-ray diffractometer and an automatic organic synthesis system will be introduced at the end of FY2023 We hope that this program will successfully be performed and equipment sharing and data sharing will be accelerated.

Ministry of Education, Culture, Sports, Science and Technology (MEXT)
Advanced Research Inftrastructure for Materials and Nanotechnology in Japan (ARIM)



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
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	T. Yokoyama	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	

(c) "Development of Cold-Atom Based Quantum Simulators and Their Applications to Quantum Computing" within the Framework of Japan's Flagship Program on Quantum Sciences and Technologies "Q-LEAP" by MEXT and "PRISM" by the Cabinet Office of Japan (2018–2028)

Quantum science and technology, such as quantum computers, quantum simulators, and quantum sensors, are qualitatively new technologies that take advantage of the "wave nature" of electrons and atoms. Since quantum science and technology can revolutionize functional materials, drug design, information security, artificial intelligence, *etc*., huge investments are being made in the science and technology policies of various countries around the world. In Japan, the "Committee on Quantum Science and Technology" was established in June 2015 by the Ministry of Education, Culture, Sports, Science and Technology to discuss policy issues related to quantum science and technology, and a new national project, the "MEXT-Quantum Leap Flagship Program (MEXT Q-LEAP)" was launched in 2018 based on the discussions held in the committee. This program is a research and development program that aims for discontinuous solutions (Quantum leap) to important economic and social issues by making full use of quantum science and technology (https://www.jst.go.jp/stpp/q-leap/en/index.html). The program consists of three technological areas: (1) Quantum information technology (Quantum simulator, Quantum computer), (2) Quantum metrology & sensing, and (3) Next generation laser.

In the ongoing research project "Development of cold-atom based quantum simulators by optical control with precisions on the attosecond temporal and nanometer spatial scales and their applications to quantum computing," which has been adopted as a Large-Scale Basic Foundation Research project in the Q-LEAP "Quantum information technology" area, the project aims to develop a completely new quantum simulator / quantum computer with core competences, which will cut deeply and sharply into fundamental problems of quantum mechanics, in close collaboration with Hamamatsu Photonics Central Research Laboratory, Kyoto University, Okayama University, Kindai University, University of Oxford, Heidelberg University, University of Strasbourg, University of Innsbruck, and others.

(d) "Large-Scale and High-Coherence Fault-Tolerant Quantum Computer with Dynamical Atom Arrays" Supported by the Cabinet Office / JST Program "Moonshot Goal 6": Realization of a Fault-Tolerant Universal Quantum Computer That Will Revolutionize Economy, Industry, and Security by 2050

The "Moonshot R&D Program" is a large-scale national research program led by the Cabinet Office, aiming to create disruptive innovations originating in Japan to address important social issues such as the super-aging society and global warming, and to promote the realization of ambitious goals "Moon Shots." (Cabinet Office/JST Moonshot R&D Program: https://www.jst.go.jp/moonshot/en/)

Goal 6, "Realization of a fault-tolerant universal quantum computer that will revolutionize economy, industry, and security by 2050," aims to develop a quantum computer that can meet the exploding demand for information processing, while conventional computers are reaching their limits in terms of progress. The key to solving diverse, complex, and large-scale real-world problems with quantum computers is the realization of a fault-tolerant universal quantum computer that can correct quantum errors during computations.

In the R&D program "Large-scale and high-coherence fault-tolerant quantum computer with dynamical atom arrays" under Goal 6, we are developing the implementation of dynamic qubit arrays in which each of the cooled atomic qubits arranged in a large array of optical tweezers is freely and rapidly moved, and gate operations, error detection and correction are carried out, as well as the implementation of a quantum computer with a quantum error-correction functionality. The goal is to realize a fault-tolerant quantum computer by achieving high stability and usability through integration and packaging of the components under the collaboration of industry and academia.

Joint Studies Programs

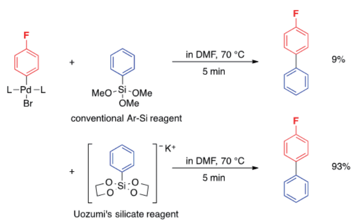
As one of the important functions of an inter-university research institute, IMS facilitates joint studies programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and 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. In the last year, we have measured the carbon K-edge NEXAFS spectrum of 100 mM trimethoxy(phenyl)silane (Ph-Si(OMe)$_3$) in tetrahydrofuran (THF) at BL3U of UVSOR-III Synchrotron, and the C–Si bond length of several organosilicon compounds were related to the reaction mechanism of Hiyama coupling reaction (by Okumura, Nagasaka, Uozumi). In this year, we have developed 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 1). Figure 2 shows the soft X-ray transmission of the developed polymer film in the soft X-ray region from 50 eV to 560 eV. Since the polymer film includes the C=C and C=N groups, the sharp absorption peaks are observed at the C and N K-edges. Since the polymer film includes no Si atoms, there is no peaks at the Si L-edge (100 eV). Soft X-ray transmission of the polymer film shows a still high value below 200 eV, indicating the developed polymer film is suitable to measure XAS of liquid in the low-energy region. By using this measurement system, we 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.

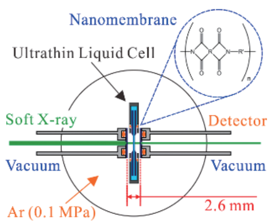


Figure 1. The schematic of an ultrathin liquid cell including Si-free nanomembranes.

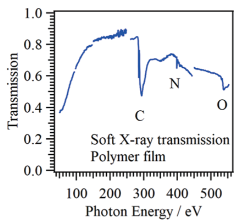


Figure 2. Soft X-ray transmission of the polymer film.

(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 by nonlinear optical spectroscopy. In particular, we conducted *operando* measurement of second-harmonic generation (SHG) and third-harmonic generation (THG) using the home-made electrochemical spectroscopic cells and systems. Then, we found that the SHG signal is highly sensitive to microscopic structural changes and degradation of the electrode surfaces in response to the applied bias voltage, whereas the electronic non-resonant THG signal is almost unaffected by structural changes on the electrode surfaces. Using SHG, we succeeded in investigating not only the oxidation process of electrode, but also the adsorption of ion and the subsequent rearrangement of interfacial water molecules. Moreover, we have succeeded in newly developing highly sensitive coherent Raman spectroscopy technique. We are also applying this new method to the observation of working electrode surfaces under reaction conditions.

Reference

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

(2) Research Symposia

(From Oct. 2022 to Sep. 2023)

Dates	Theme	Chair
Nov. 8, 2022	Resonant Soft X-Ray Scattering and Reflectivity: Nano/Mesoscale Structural Analysis of Soft Materials and Soft Matter	**ARAKI, Tohru** **KERA, Satoshi**
Nov. 28, 2022	Conference on Generation and Advanced Applications of Various Quantum Beams in UVSOR-III	**TAIRA, Yoshitaka**
Mar. 29–30, 2023	Understanding and Design of Biomolecular Machinery: Next Challenges of Molecular Engine	**UENO, Takafumi** **IINO, Ryota**
Jun. 14–15, 2023	Industry-Academia-Government-Citizens Collaboration for a Sustainable Society with Examples from Chemistry, Engineering, and Environmental Studies	**TOKORO, Chiaru** **OKAMOTO, Hiromi**
Jul. 29–30, 2023	Seeds and Needs for Tomorrow's Synchrotron Radiation Photoelectron Spectroscopy Research	**MATSUI, Fumihiko**
Aug. 31, 2023	Morino Discussion	**MUNAKATA, Toshiaki** **KURAMOCHI, Hikaru**
Sep. 13–14, 2023	Toward the Development of Ionic Liquid Informatics	**KITADA, Atsushi** **KERA, Satoshi**
Sep. 29, 2023	UVSOR–SPring8 Infrared Beamline Joint Users Meeting	**TANAKA, Kiyohisa**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2022–Mar. 2023		Apr. 2023–Sep. 2023		Total		
		Regular	ARIM	Regular	ARIM	Regular	ARIM	Sum
Special Projects		2		1		3		3
Research Symposia		3		5		8		8
Research Symposia for Young Researchers		0		0		0		0
Cooperative Research		25	25	17	22	42	47	89
Use of Facility	Instrument Center		75		70		145	145
	Equipment Development Center	0	7	0	5	0	12	12
	UVSOR	105	3	104	1	209	4	213
Use of Facility Program of the Computer Center						298*		298*

* from April 2022 to March 2023

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. 1–2026. 1	6	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2009.10–2024.10	8	0
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	1	0
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. 6–2028. 5	1	1
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	2	1
Fritz-Haber-Institut der Max-Planck-Gesellschaft [Germany]	2021. 4–2023. 3	0	0
China Scholarship Council [China]	2023. 1–2028. 1	0	0

* No. of researchers during the period from Oct. 2022 to Sep. 2023

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	3	1
Vidyasirimedhi Institute of Science and Technology [Thailand]	2018. 9–2023. 9	0	0
Friedrich Schiller University Jena [Germany]	2020. 7–2023. 7	0	2
Chulalongkon University [Thailand]	2010. 4–2027. 9	1	2

* No. of researchers during the period from Oct. 2022 to Sep. 2023

(2) IMS International Internship Program

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	32*	–

* from Oct. 2022 to Sep. 2023

(3) IMS International Collaboration (Including online meetings)

Category	Number of People
International Joint Research Programs	82
International Use of Facilities Programs	31

from Oct. 2022 to Sep. 2023

Internationally Collaborated Publications

Articles and reviews published in 2022

Underlined countries include MOU Partnership Institutions
Scopus dataset, Oct. 2023