Special Research Projects

IMS has special research projects supported by national funds. Five 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 R&D Program "Moonshot Goal 6": Realization of a Fault-Tolerant Universal Quantum Computer That Will Revolutionize Economy, Industry, and Security by 2050

(e) MEXT Promotion of Development of a Joint Usage/Research System Project: Coalition of Universities for Research Excellence Program (CURE): Frontier of Spin Life Sciences [Spin-L]

These five 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

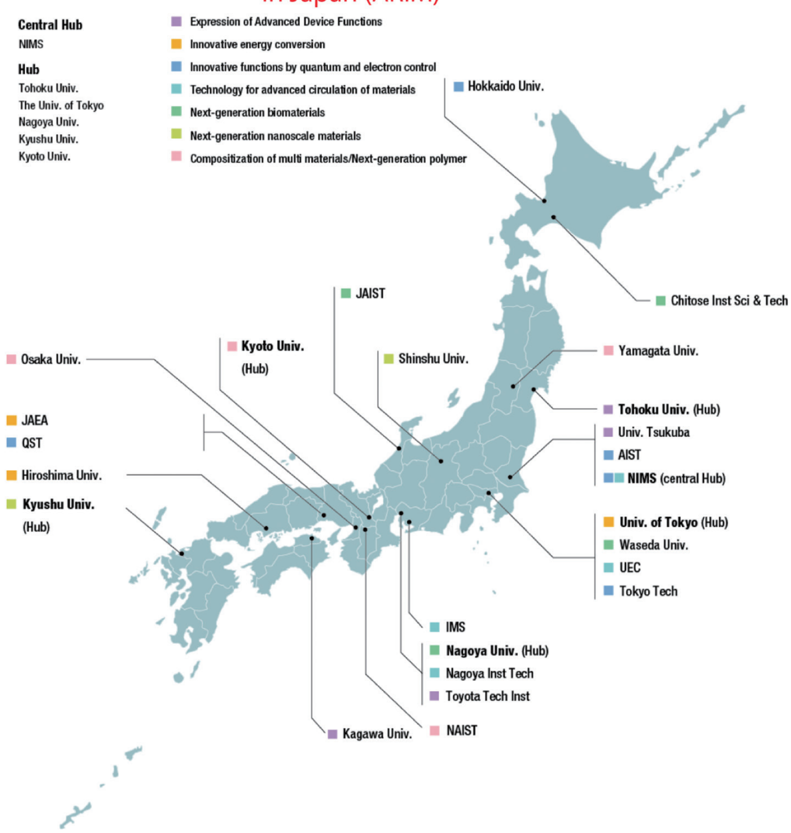
It is highly important to improve instrumental supporting environments for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting researches and educations with high standard quality. To install such sophisticated instruments, 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 19,500 in 674 universities/institutions/companies (as of July, 2024). Network usage reaches more than 190,000 times a year, in which external usage amounts to 5,400 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 Infrastructure for Materials and Nanotechnology in Japan) program supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT) 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 "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. 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 D Platform" in collaboration with the Data creation/utilization type material research and development 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. Through this program, a new electron spin resonance (ESR) system and a new superconducting quantum interference device (SQUID) magnetometer were installed in IMS in 2021 and 2022, and a high-throughput low-temperature single-crystal x-ray diffractometer and an automatic organic synthesis system were introduced in 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 (FY2023)

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
UVSOR Synchrotron Radiation	X-Ray Magnetic Circular Dichroism	T. Yokoyama	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		M. Fujiwara, M. Miyajima
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	Y. Furuike
	Molecular Structure Analysis using Crystalline Sponge Method	M. Fujita	T. Mitsuhashi, T. Yokoyama
Electron Spectroscopy	X-Ray Photoelectron Spectroscopy	T. Yokoyama	S. Iki, 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	
	Magnetic Thin Films	T. Yokoyama	
	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 (MEXT) 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 by the committee. This 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.

The ongoing research project led by Prof. Kenji Ohmori at IMS and named "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, 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 Kyoto University, Okayama University, and Kindai University.

(d) "Large-Scale and High-Coherence Fault-Tolerant Quantum Computer with Dynamical Atom Arrays" Supported by the Cabinet Office / JST R&D 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 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.

The R&D project "Large-scale and high-coherence fault-tolerant quantum computer with dynamical atom arrays" led by Prof. Kenji Ohmori at IMS under Goal 6 develops dynamical qubit arrays in which each of the cold-atom qubits arranged in a large array of optical tweezers is freely and rapidly moved during computation including gate operations and error detection / correction. The goal is to realize a practical fault-tolerant quantum computer with high stability and usability through integration and packaging of the key components under the collaboration with industries.

(e) MEXT Promotion of Development of a Joint Usage/Research System Project: Coalition of Universities for Research Excellence Program (CURE): Frontier of Spin Life Sciences [Spin-L]

Spin-L

Frontier of Spin Life Sciences

In the MEXT CURE project, we form a new system for collaborating with research institutions and research communities that are different from conventional ones to advance research in interdisciplinary fields where research systems have not yet been established. The hub is based on the accumulation of joint usage/research systems that have been formed based on the centrality of specific fields.

The MEXT CURE project Frontier of Spin Life Sciences [Spin-L] started in September 2023. In order to develop a new field that combines molecular science, life science, and physiological science, we will establish "Frontier of Spin Life Sciences," which brings together the basic technology of magnetic resonance (MR) equipment and researchers across disciplines.

The three Okazaki institutions (NIPS, IMS, ExCELLS) form the core, and are working together to develop new molecular probes for MR and perform MR image measurements on model animals. We explore new principles and methods for MR measurements on living organisms. In order to strongly develop this cutting-edge research by bringing together researchers in related fields in Japan, we will promote industry–academia collaborative research using project research by specially appointed faculty and cross-appointments, human exchange, joint usage/research, and human resource development with companies at the Under One Roof on Okazaki Campus.

For technologies and compound synthesis that are not specialized in the three Okazaki institutions, Institute for Chemical Research (Kyoto University), Institute for Protein Research (Osaka University), Brain Research Institute (Niigata University), and Institute for Quantum Life Science (QST) collaborate as participating institutions to promote the project. This project not only promotes joint usage/research through collaboration with many universities, companies, and various equipment platforms and field communities, but also aims to train cross-disciplinary researchers and technical staff.

Main achievements in FY2023

(1) Establishment of management system:

Signed a memorandum of understanding regarding the operation of Spin-L Hub, *etc.* (core/node organization). Established operating rules. Established and held core meetings, hub meetings, and steering committees. Strengthened the management office. Assigned a full-time URA. Established the Spin-L logo mark. Held kickoff meeting.

(2) Promotion of joint usage/research:

Established "joint usage/joint research committee." Started spin-life joint utilization research (46 projects conducted).

(3) Human resource development:

Established the "interdisciplinary association of young researchers." Held 5 Co-sponsored seminars.

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) Establishing a Unified Picture of Multiscale Quantum Functions in Chiral Materials

KISHNE, Jun-ichiro (*Open Univ.*)
TOGAWA, Yoshihiko (*Osaka Metropolitan Univ.*)
SATO, Takuya (*Tokyo Inst. Tech.*)
KUSUNOSE, Hiroaki (*Meiji Univ.*)
KATO, Yusuke (*Univ. Tokyo*)
YAMAMOTO, Hiroshi (*IMS*)

The term “chirality” refers to forms that are mirror images of each other but cannot be superimposed, like right and left hands. As a term describing molecular shapes, it has become widely recognized across various branches of molecular science. A noteworthy point is the subtle connection between macroscopic hands and microscopic molecules, both referred to by the same term, “chirality.” This connection raises an important question: How can the macroscopic classical world and the microscopic quantum world be linked? One of the key goals for material science researchers is to explore material functions on multiple scales and bridge these two realms. The analogy between “molecules and hands” illustrates the multiscale nature of chirality. Under this common keyword “chirality,” vast research fields are expanding, spanning physics, chemistry, life sciences, and even space science. Chirality serves as a unifying concept across these disciplines.

The reason we focus on chirality is that while it may appear to be a geometric and static concept, chirality actually connects quantum degrees of freedom, such as charge, orbit, spin, and lattice vibrations, leading to a wealth of material functions. To use a familiar analogy, when ascending or descending a spiral staircase, one inevitably rotates around the helical axis. In other words, translation and rotation are coupled. Applying this perspective to materials reveals that electrical and magnetic degrees of freedom are similarly coupled.

Recently, the field of “chiral material science,” which explores the structure and function of materials from this perspective, has emerged. Fields such as chiral magnetism, chiral plasmonics, chiral spintronics, chiral phononics, chiral optics, and chiral electronics are all emerging areas that are very active today. If you remove the prefix “chiral” from the names of these fields, you find they encompass nearly the entirety of physics and chemistry.

The goal of this research project was to bring together six researchers—three experimentalists and three theorists—who are fascinated by chirality, to investigate how microscopic quantum mechanical degrees of freedom, such as electron spin, orbit, and atomic vibrations, couple in chiral materials. Using techniques such as circularly polarized Raman spectroscopy and spin-polarized transport measurements, we have studied the chiral responses of a wide range of materials, including organic and inorganic compounds, conductors, semiconductors, dielectrics, bulk crystals, and thin films. These experimental investigations have been complemented by theoretical research.

Several significant achievements have emerged from this research. We successfully observed lattice vibrations (phonons) unique to chiral crystals using circularly polarized Raman scattering and identified the quantum numbers of phonons derived from chirality through Raman selection rules (Sato, Kishine, Togawa *et al.*, *Nat. Phys.* **19**, 35–39 (2023)). In addition, we discovered that applying a thermal gradient to quartz, a representative chiral inorganic crystal, induces a spin current, a previously unobserved phenomenon (Togawa *et al.*, *Phys. Rev. Lett.* **132**, 056302 (2024)). We also proposed a theoretical framework for defining chirality in quantum terms (Kusunose, Yamamoto, Kishine, *Israel J. Chem.* **62(11-12)**, e202200049 (2022); *Appl. Phys. Lett.* **124**, 260501 (2024)).

These studies, while seemingly diverse, all relate to elucidating the phenomenon where the spins of electrons passing through chiral molecules or crystals exhibit huge spin polarization. This phenomenon, known as Chirality-Induced Spin Selectivity (CISS), was first discovered by Naaman’s group in Israel. CISS occurs on multiple scales, from DNA and peptides to inorganic crystals, and aligns electron spins without the need for a magnetic field, even at room temperature. This makes it a highly attractive phenomenon, and understanding its mechanism is a profoundly important scientific goal. All of the results from this project are critical steps towards unraveling the CISS mechanism.

To further advance this research, we have established the “Quantum Mechanical Research Initiative for Chiral Materials (QuaRC)” at the Institute for Molecular Science (IMS) (https://www.quarc-ims.com/). Leveraging IMS as a joint-use facility, we aim to develop this initiative into a consortium that promotes chirality research from both the physical and chemical perspectives.

Finally, we stress that brainstorming and refining ideas often become a lengthy process, much like an endurance race in front of the whiteboard, requiring in-depth, face-to-face interaction. A key achievement during this research period was the regular in-person meetings in Okazaki, where the six team members gathered multiple times for productive discussions.

(2) Research Symposia

(From Oct. 2023 to Sep. 2024)

Dates	Theme	Chair
Oct. 2–4, 2023	Frontier of Soft X-Ray Spectroscopy for Chemical Processes in Solutions	**NAGASAKA, Masanari** **KERA, Satoshi**
Aug. 19–23, 2024	The 63rd Summer School in Molecular Science	**TANAKA, Ryoichi** **SUGIMOTO, Toshiki**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2023–Mar. 2024		Apr. 2024–Sep. 2024		Total		
		Regular	ARIM	Regular	ARIM	Regular	ARIM	Sum
Special Projects		1		0		1		1
Research Symposia		1		0		1		1
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		16	28	18	26	34	54	88
Use of Facility	Instrument Center		98		73		171	171
	Equipment Development Center	0	5	0	6	0	11	11
	UVSOR	87	2	118	1	205	3	208
Use of Facility Program of the Computer Center						302*		302*

* from April 2023 to March 2024

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	7
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2005. 1–2026. 1	0	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2009.10–2029.10	7	1
Freie Universität Berlin (FUB) [Germany]	2013. 6–2025. 6	0	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. 5–2027. 5	0	0
National Yang Ming Chiao Tung University [Taiwan]	2018. 6–2028. 5	3	0
Peter Grünberg Institute, Forschungszentrum Jülich GmbH (FZJ) [Germany]	2018.10–2028. 9	0	1
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. 4–2026. 3	0	4
China Scholarship Council [China]	2023. 1–2028. 1	2	0

* No. of researchers during the period from Oct. 2023 to Sep. 2024

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

Institution	Period	Accept*	Send*
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2026. 3	3	3
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2024.11	4	2
Vidyasirimedhi Institute of Science and Technology [Thailand]	2018. 9–2028. 9	0	0
Friedrich Schiller University Jena [Germany]	2020. 7–2028. 7	1	0
Chulalongkon University [Thailand]	2010. 4–2027. 9	5	4

* No. of researchers during the period from Oct. 2023 to Sep. 2024

(2) IMS International Internship Program

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	27*	–

* from Oct. 2023 to Sep. 2024

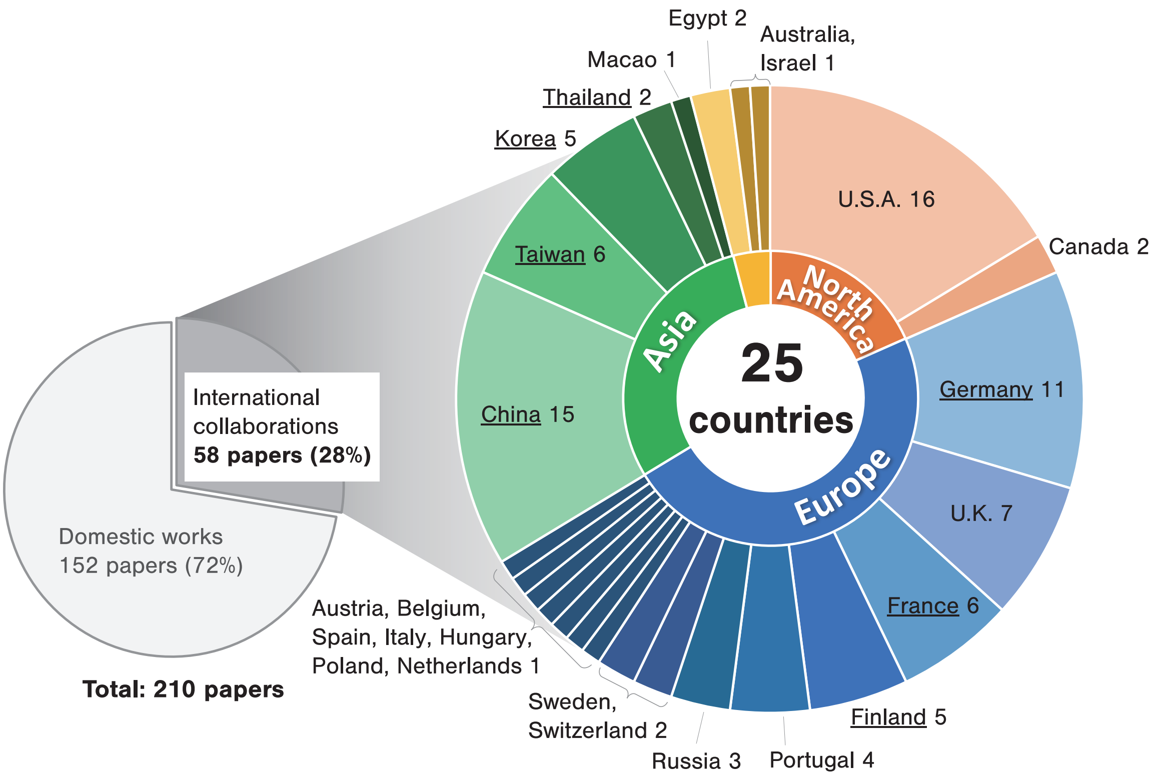
(3) IMS International Collaboration (Including online meetings)

Category	Number of People
International Joint Research Programs	97
International Use of Facilities Programs	40

from Oct. 2023 to Sep. 2024

Internationally Collaborated Publications

Articles and reviews published in 2023



Underlined countries include MOU Partnership Institutions
Scopus dataset, May 2024