

Special Research Projects

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

- (a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT)
Flagship 2020 Project, Priority Research 5
“Development of New Fundamental Technologies for Highly-Efficient Energy Creation, Conversion, Storage, and Use”
- (b) MEXT Nanotechnology Platform Program
Platform of Molecule and Material Synthesis
- (c) Inter-University Network for Efficient Utilization of Research Equipments
- (d) Consortium for Photon Science and Technology (C-PhoST)

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) The Ministry of Education, Culture, Sports, Science and Technology (MEXT) Flagship 2020 Project, Priority Research 5 “Development of New Fundamental Technologies for Highly-Efficient Energy Creation, Conversion, Storage, and Use”

A new supercomputer, post-K computer, is being developed by RIKEN as a successor to the K computer. This will help solve various social and scientific problems. Nine priority research fields were defined by the government and the application software for them is also being developed. Among them, IMS is responsible to the priority research 5, “Development of New Fundamental Technologies for Highly-Efficient Energy Creation, Conversion, Storage, and Use.” IMS organizes a network project group with Kobe University, RIKEN, the University of Tokyo, National Institute for Material Science (NIMS), Nagoya University, Okayama University, Hokkaido University, and Waseda University in corporation with 46 institutions including 14 companies.

The highly integrated computer resources of the post-K computer will allow us to expand our current research across many disciplines. Realistic simulations will be made possible at the electronic and molecular scales, and will help us gain the details of chemistry and physics in complex compounds that play substantial roles in solar energy reactions and electrochemical processes.

We propose to perform these state-of-the-art calculations to unravel the following issues; Branch A: Production and storage of alternative energy sources with solar cells and artificial photosynthesis; Branch B: Conversion and storage of energies produced in fuel cells and rechargeable batteries; Branch C: Separation, recovery, and storage of methane and

CO₂; effective use of energies and resources produced by catalytic reactions. We are also collaborating with experimental researchers and industries to establish new energy technologies that are highly efficient, low cost, environmentally clean, and sustainable.

Due to the restriction in computer resources, computational researches have been typically limited to the investigation of isolated and/or partial systems to provide only one aspect of the entire system. The post-K computer is powerful enough to make such calculations obsolete; it will open new frontiers and establish new academic standard in computational chemistry and physics, enabling the understanding of fully complex physics associated with interfaces of real materials as well as inhomogeneous electrons and molecules.

In FY2015, we organized an advisory committee containing seven members: Three experimental researchers, two computational scientists, one computer scientist, and one senior researcher from industry. Then we held meetings of this committee on October 20, 2015, and January 4, 2016 where we explained and discussed the research plan of the project. The second open symposium of the project was held on March 7, 2016. Many researchers participated in the symposium and joined the discussions. Finally we refined the research and development plan of the project and submitted it to MEXT. We plan to keep similar activities during the project period.

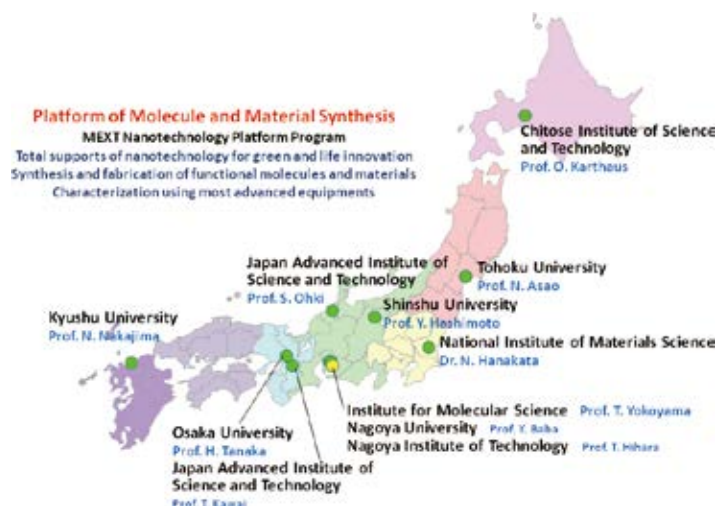


K computer being used by Priority Research 5.

(b) 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 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 constitutes 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 univer-

sities 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 FY2015 amounted 170 (161 non-proprietary and 9 proprietary proposals, excluding applications from IMS) and the total number of days used for the supports is 3113 (3065 days for non-proprietary proposals and 48 days for proprietary ones).



List of Supports in IMS (FY2015)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	Y. Kaneko, M. Inoue, Y. Funaki, J. Aoki, M. Yokota, N. Nakagawa, A. Ota
Organization Management in IMS			
UVSOR Synchrotron Radiation	Scanning Transmission X-Ray Microscopy	N. Kosugi	T. Ohigashi, Y. Inagaki
	X-Ray Magnetic Circular Dichroism	T. Yokoyama	Y. Takagi, M. Uozumi, Y. Uemura
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Suzui, M. Aoyama, N. Takada, T. Kondou
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Aoyama, H. Yoshida
Electron Microscopy	300kV Transmission Electron Microscopy	T. Yokoyama	T. Ueda, S. Iki
	Field Emission Scanning Electron Microscopy		S. Nakao
	Low vacuum Analytical Scanning Electron Microscopy		S. Nakao, M. Sakai
Focus Ion Beam Processing	S. Nakao		
X-rays	Single Crystal X-Ray Diffractometer		M. Fujiwara
	Single Crystal X-Ray Diffractometer for Microcrystals	Y. Okano	
	Powder X-Ray Diffractometer	M. Fujiwara	
	X-Ray Fluorescence Analysis	T. Ueda, S. Iki	
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama

Electron Spectroscopy	Electron Spectroscopy for Chemical Analysis	N. Kosugi	M. Sakai
	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	N. Kosugi, S. Kera, K. Tanaka	H. Yamane, S. Ideta
Electron Spin Resonance	Pulsed High Field ESR	T. Nakamura, T. Yokoyama	M. Fujiwara
	X-Band CW ESR		
	X, Q-Band CW ESR		
SQUID	Superconducting Quantum Interference Device		M. Fujiwara
Thermal Analysis	Differential Scanning Calorimeter (Solutions)		S. Makita, H. Nagao
	Isothermal Titration Calorimeter (Solutions)		M. Fujiwara
	Calorimeter for solids		S. Makita
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		S. Makita
Spectroscopy	Microscopic Raman Spectroscopy	T. Yokoyama	M. Uruichi
	Fourier Transform Far Infrared Spectroscopy		T. Ueda
	Fluorescence Spectroscopy		S. Makita
	Ultraviolet & Visible Absorption Spectroscopy		T. Ueda
	Circular Dichroism		T. Yamanaka
Lasers	Picosecond Laser		T. Ueda
	Nanosecond Excimer/Dye Laser		
	Nanosecond Nd:YAG OPO Laser		T. Yamanaka
	Nanosecond Fluorinated Excimer Laser		
High Field NMR	920 MHz NMR Solutions & Solids	K. Kato, K. Nishimura, T. Yokoyama	K. Okushita
	800 MHz Solutions, Cryostat Probe	K. Kato	T. Yamaguchi
	600 MHz Solids	K. Nishimura	K. Okushita
	600 MHz Solutions	T. Yokoyama	S. Makita, H. Nagao
Functional Molecular Synthesis and Molecular Device Fabrication	Organic Thin Film Solar Cells	M. Hiramoto	
	Organic Field Effect Transistors	H. Yamamoto	M. Suda
	Functional Organic Synthesis	T. Yokoyama	S. Higashibayashi
	Large Scale Quantum Mechanical Calculations	M. Ehara	R. Fukuda
	Magnetic Thin Films	T. Yokoyama	Y. Takagi, M. Uozumi, Y. Uemura
	Metal Complexes	S. Masaoka	M. Kondo
	Inorganic Materials	G. Kobayashi	

(c) 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 5 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. 73 national universities all over Japan have been participating in the network. They are grouped into 12 regions and in each region the regional committee discusses and determines the operation of regional

network system 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 every public and private university. Since 2010, the project has been renamed "Inter-University Network for Common Utilization of Research Equipments" still keeping the original strategy and stable functioning. In August 2016, the number of user registrants amounts to 10,821 in 211 universities/institutions/companies covering 2,594 laboratories in Japan. Usage of the network reaches almost 10,000 times per month and keeps growing in numbers. We are now planning to reconstruct a new reservation and charging system that will be more user-friendly and convenient. Moreover, we will actively provide various opportunities where technical staffs and users can improve their technical skills and frankly communicate with each other.

(d) Consortium for Photon Science and Technology (C-PhoST)

In order to establish strong bases in the research and education in optical science, a 10-year program “Photon Frontier Network” has been started in 2008 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). Consortium for Photon Science and Technology (C-PhoST) is the one of two research consortia of Photon Frontier Network. It is composed of 4 Core Organizations headed by Principal

Investigators (written in parentheses): Osaka University (R. Kodama), Kansai Photon Science Institute (K. Kondo), Kyoto University (S. Noda) and Institute for Molecular Science (K. Ohmori). The major strength of this Consortium is the collaboration among the specialists in three fields: high power lasers, photonic crystals, and coherent control.

Okazaki Conference

The 75th Okazaki Conference Tensor Network States: Algorithms and Applications 2016

(January 11–14, 2016)

Organizers: T. Nishino (*Kobe Univ.*), G. Vidal (*Perimeter Inst. Theor. Phys., Canada*), Y.-J. Kao (*Natl. Taiwan Univ., Taiwan*), T. Xiang (*IPCAS, China*), C. Hotta (*Univ. Tokyo*), T. Hikihara (*Gumma Univ.*), K. Okunishi (*Niigata Univ.*), S. Todo (*Univ. Tokyo*) and Y. Shikano (*IMS*)

Invited Speakers: T. Yanai (*IMS*), N. Nakatani (*Hokkaido Univ.*), G. Chan (*Princeton Univ., U.S.A.*), A. Sandvik (*Boston Univ., U.S.A.*), G. Vidal (*Perimeter Inst. Theor. Phys., Canada*), Y.-J. Kao (*Natl. Taiwan Univ., Taiwan*), T. Xiang (*IPCAS, China*), T. Okubo (*Univ. Tokyo*), F. Pollmann (*MPIPKS, Germany*), Y. Ran (*Boston Col., U.S.A.*), H. Imai (*Univ. Tokyo*), D. Poilblanc (*CNRS and Univ. Toulouse, France*), M. C. Banuls (*MPQ, Germany*), S. Yang (*Perimeter Inst. Theor. Phys., Canada*)

Tensor networks are recognized as one of the most promising numerical tools to study quantum many body systems; representatives are the matrix product state (MPS), the multi-scale entanglement renormalization ansatz (MERA), and the projected entangled-pair states (PEPS), and Density Matrix Renormalization Group (DMRG). By now, the concept covers various fields including material science, quantum chemistry, and lattice gauge theories, and it is desired to share ideas among these fields.

This workshop focused on the recent developments on tensor network based algorithms and applications. It hosted the discussion of current problems and developments among the leading researchers, aiming to promote interactions between selected fields from statistical mechanics to condensed matter, from quantum chemistry to nano-technology and high energy physics.



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. The Third Phase of π -Electron-Based Solid State Science

KATO, Reizo (*RIKEN*)
 NAKAZAWA, Yasuhiro (*Osaka Univ.*)
 OGATA, Masao (*Univ. Tokyo*)
 UJI, Shin-ya (*NIMS*)
 TERASAKI, Ichiro (*Nagoya Univ.*)
 YAMAMOTO, Hiroshi (*IMS*)

Recently, physical properties of molecule-based π -electron systems are attracting much attention not only because of the advancement in organic electronics such as OLED (= organic light-emitting-diode), OFET (= organic field-effect-transistor), and OPV (= organic photovoltaics) but also because of the discovery of advanced functionality such as electronic ferroelectrics, superconducting transistors, electron glass, quantum spin-liquid, and light-induced ultrafast phase transitions. Those new phenomena sometimes requires researchers to reconsider their way of understanding on electronic states in solids, because they seem to be emerging from spatiotemporal inhomogeneity that has not been seriously considered before (Figure 1). Therefore, it is highly demanded to develop new methods that allow us to understand and control the new states of electrons in terms of both experimental and theoretical solid state physics. Historically, the development of π -electron-based material has started from establishing the concept of 'organic semiconductors' by Prof. Inokuchi and it was followed by syntheses of many organic materials that exhibit metallic and even superconducting phases. After this first phase of material development, the second phase of π -electron material development has been led by physicists and physical chemists who have discussed band structures with coherent electrons, which had been hardly believed to exist in organics before those studies. In this context, we are now at the starting point of the third phase of π -electron-based solid state science. This new era requires researchers to develop new methods in all aspects of material development, observation/analytical method, and theoretical understanding. At the same time, it is necessary to facilitate interdisciplinary interaction among physicists, chemists, and device technologists to tackle this problem. This project aims at promoting such interdisciplinary discussions by holding a workshop with wide range of participants who share the common issues from different points of view.

During the workshop, it was recognized that the competition among energies with similar strengths can result in a situation of high complexity, yet such a complexity can generate unprecedented and interesting phenomena. In molecu-

lar materials, the energies of electron's motion, lattice, spin, and Coulomb interaction are at similar extent, and therefore mix together to form inhomogeneous but hierarchical structures in space and time domains. Theories now available seem to fail to help researchers understand and control such entangled situations. The participants agreed on the importance of developing new theories based on non-periodic structures, although complete removal of the periodicity is hard to be considered. The participants also agreed to continue this type of discussion and to propose a new research field that might be able to be called 'quantum π -ology'. Such a new science should result in understanding and control of strong correlation, glassy state, non-equilibrium state, frustrated state, and ultra-fast transitions of π -electron systems in future. This project has succeeded to launch such a new research community that will pave the way to the third phase of π -electron science.

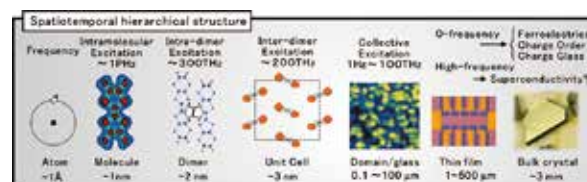


Figure 1. Spatiotemporal hierarchical structure of electrons and lattices in π -electron systems.

B. Catalysis Based on the Elemental Strategy

UOZUMI, Yasuhiro (*IMS*)
 NAKAMURA, Masaharu (*Kyoto Univ.*)
 KAKIUCHI, Fumitoshi (*Keio Univ.*)

Adhoc members
 MURAI, Shinji (*Nara Inst. Sci. Tech.*)
 TAMAO, Kohei (*RIKEN*)
 MOMIYAMA, Norie (*IMS*)
 OSAKO, Takao (*IMS*)
 HAMASAKA, Go (*IMS*)

Rare resources, represented by rare earth and other rare metal elements which are being utilized for the advanced industries are facing their price increase and tight supply due to rapid increase of their consumptions and producing countries' resource management policies accompanying with the global economic growth and advanced industries' expansion.

In the past several decades, transition metal catalyses have been playing key role in the chemical industries to realize efficient organic molecular transformations, and rare and

noble transition metals (*e.g.* Pd, Pt, Rh, *etc.*) are often utilized as the central elements of the catalysts. Taking into accounts the above mentioned situations of elemental strategies, development of novel catalytic processes without rare and noble metals have been rapidly becoming an eagerly awaited research subjects.

This special project entitled “Catalysis Based on the Elemental Strategy” started in 2015 (one-year project) as a feasibility study to launch national-size research project of catalysis based on the elemental strategy. The three main proposers organized a study group by which the feasibility study meetings were held 3 times in 2015 (9th–10th of January (at Atami), 19th–20th of July (at Toyama), and 10th October (at Okazaki)), and once in 2016 (23rd–24th January (at Yamaguchi)).

Among them, the meetings at Atami, Toyama, and Yamaguchi were held with some adhoc members, as a concomitant meeting of JST-CREST meeting on Elemental Strategy (a representative: Prof. Kohei Tamao).

Through the thorough discussion on the feasibility, this study group decides to make proposals of a couple of research projects related to this special project to MEXT and/or JSPS. Thus, a research project on developing an analytical system for elucidating the catalytic reactions utilizing synchrotron light sources *etc.* and that on developing novel catalytic systems, which would realize elemental-replacement, elemental-circulation, as well as elemental-reduction, will be proposed in due course.

(2) Research Symposia

(From Oct. 2015 to Sep. 2016)

Dates	Theme	Chair
Oct. 22, 2015	Workshop of Theoretical and Computational Molecular Science: Development of Computation Methods and Simulations	YANAI, Takeshi
Nov. 27, 2015	Emergence of Interaction and Hierarchy Hidden in Data	HIRA, Ri-ichiro SHIKANO, Yutaka
Feb. 11–12, 2016	Current and Future Status of Bright and Intense Infrared Light Source	ZEN, Heishun KATOH, Masahiro
Feb. 15–17, 2016	Japan-Korea Seminars on Biomolecular Science: Experiments and Simulation	AONO, Shigetoshi
Feb. 23–26, 2016	Japan-China Joint Symposium on Functional Supramolecular Architectures	MAEDA, Hiromitsu JIANG, Donglin
Mar. 5– 6, 2016	Materials Engineering Science with Asymmetric Coordination Sphere Design and Anisotropic Integration of Metal Complex	SHIONOYA, Mitsuhiko MASAOKA, Shigeyuki
Mar. 9–10, 2016	Molecular Catalysis Science: Interplay between Theory and Experiment	HASEGAWA, Jun-ya EHARA, Masahiro
Jun. 27–28, 2016	Engineering Super-Functional Molecules: Strategy for Design and Development of Socially Implementable Molecules Achieved by Cooperation among Synthesis, Measurement and Mathematical Analysis	UENO, Takafumi IINO, Ryota
Sep. 2– 3, 2016	Major Trends in Organometallic Chemistry	HIRATA, Shuichi UOZUMI, Yasuhiro
Sep. 29– 30, 2016	Japan-Korea-Taiwan Joint Symposium on Bioinorganic Chemistry	AONO, Shigetoshi
Jun. 26, 2016	Meeting for Lectures at 56 th Summer School on Molecular Science for Young Scientists	MIZUNO, Yuta FURUTANI, Yuji
Jan. 11–14, 2016	Tensor Network States: Algorithms and Applications 2016	SHIKANO, Yutaka

PROGRAMS

(3) Numbers of Joint Studies Programs

Categories		Oct. 2015–Mar. 2016		Apr. 2016–Sep. 2016		Total		
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		0		2		2		2
Research Symposia		7		4		11		11
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		30	33	37	36	67	69	136
Use of Facility	Instrument Center	7	70		74	7	144	151
	Equipment Development Center	2	7	1	5	3	12	15
Use of UVSOR Facility		61	20	65	21	126	41	167
Use of Facility Program of the Computer Center						217*		217*

* from April 2015 to March 2016

Collaboration Programs

(a) International 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
Workshop and Colloquium "Grand Design of Molecular Systems; Dynamic, Correlation and Harmony"	OHMINE, Iwao (IMS)	2015.10.8	IMS
The Winter School of SOKENDAI	YAMAMOTO, Hiroshi (IMS) MOMIYAMA, Norie (IMS)	2015.12.1–12.4	NIFS, IMS
The 3 rd Workshop on Physics in Organic Optoelectronics	KERA, Satoshi (IMS)	2015.12.10–12.11	IMS
The 75 th Okazaki Conference "Tensor Network States: Algorithms and Applications 2016"	NISHINO, Tomotoshi (Kobe Univ.) VIDSL, Guifre (Perimeter Inst. for Theoretical Physics, Canada) KAO, Ying-Jer (National Taiwan Univ., Chinese Taiwan) XIANG, Tao (Inst. of Physics, Chinese Acad. of Sci.) HOTTA, Chisa (Univ. Tokyo) HIKIHARA, Toshiya (Gumma Univ.) OKUNISHI, Kouichi (Niigata Univ.) TODO, Synge (Univ. Tokyo) SHIKANO, Yutaka (IMS)	2016.1.11–1.14	IMS
The 4 th CU-IMS Symposium: 10 Years of Fruitful Relationship and Beyond (PACCON2016)	WACHARASINDHU, Sumrit (CU, Thailand)	2016.2.10	BITEC, Bangkok, Thailand
Korea-Japan Seminars on Biomolecular Sciences: Experiments and Simulations	AONO, Shigetoshi (IMS) IINO, Ryota (IMS) JEONG, Hawoong (KAIST) KATO, Koichi (IMS) KUWAJIMA, Kunihiko (Univ. Tokyo) LEE, Jooyoung (KIAS) YAMAGUCHI, Takumi (JAIST)	2016.2.15–2.17	IMS
KU-IMS Symposium	HANNONGBUA, Supa (KU, Thailand)	2016.6.3	Kasetsart University, Bangkok, Thailand

(b) IMS International Internship Programs and SOKENDAI International Lecture & Training Courses

Category	Number of People*	
	Overseas	Domestic
IMS International Internship Program	21	–
SOKENDAI Asian Winter School (2015.12.1–12.4)	25	5

* from Sep. 2015 to Aug. 2016

PROGRAMS

(c) IMS International Collaboration

Category	Number of People*
International Joint Research Programs	70
International Use of Facilities Programs	51

* from Sep. 2015 to Aug. 2016

(d) MOU Partnership Institutions

IMS has concluded academic exchange and 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]	2014.10–2018.10	0	0
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2014. 2–2017. 2	1	2
Institute of Chemistry Chinese Academy of Science (ICCAS) [China]	2013. 9–2018. 9	1	5
Korea Advanced Institute of Science and Technology (KAIST) [Korea]	2016. 9–2020. 9	0	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2014.10–2019.10	10	1
Indian Association for the Cultivation of Science (IACS) [India]	2013. 3–2017. 3	0	0
Freie Universität Berlin (FUB) [Germany] Helmholtz Zentrum Berlin (HZB) [Germany]	2016. 6–2019. 6	10	8
Indian Institute of Science Education and Research Kolkata (IISER Kolkata) [India]	2015. 9–2019. 8	4	0
Indian Institute of Science (IISc) [India]	2015.10–2019. 9	0	1

* from Sep. 2015 to Aug. 2016

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

Institution	Period	Accept*	Send*
Chulalongkorn University, Faculty of Science [Thailand]	2010. 4–2020. 3	10	15
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2021. 4	3	5
Mahidol University, Faculty of Science [Thailand]	2014. 3–2019. 3	2	5
Nanyang Technological University, College of Science [Singapore]	2014. 3–2019. 3	0	1
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2019. 3	2	0

* from Sep. 2015 to Aug. 2016