Special Research Projects

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

(a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT)
Flagship Project, Priority Research Issue
"Development of New Fundamental Technologies for High-Efficiency 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

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

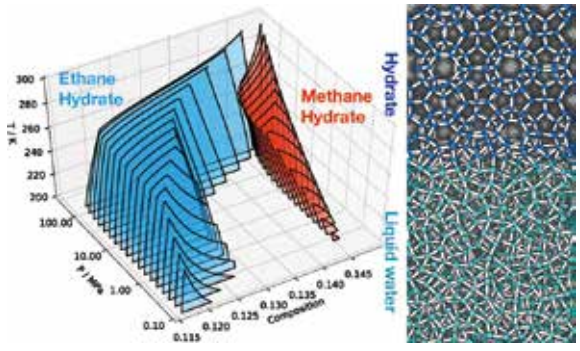
(a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT) Flagship Project, Priority Research Issue, "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use"

A new supercomputer, the so-called post-K computer (supercomputer Fugaku), is being developed by RIKEN as the successor to the K computer and is expected to help to solve various social and scientific problems. Nine priority research issues have been defined by the government, and at the same time, software development is also in progress. IMS leads one of the priority research issues, "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use" in collaboration with Kobe University, RIKEN, the University of Tokyo, the National Institute for Materials Science (NIMS), Nagoya University, Okayama University, Hokkaido University, and Waseda University, incorporating 51 institutions including 23 companies.

We propose to perform state-of-the-art calculations to unravel the following issues. Branch A: Production and storage of alternative energy sources using solar cells and artificial photosynthesis; Branch B: Conversion and storage of energy produced in fuel cells and rechargeable batteries; Branch C: Separation, recovery, and storage of methane and CO_2 and effective use of energy and resources produced by catalytic reactions. We will also collaborate with experimentalists in academia and researchers in industries to establish new energy technologies which are highly efficient, inexpensive, environmentally clean, and sustainable.

Because of the limitation of current computer performance, conventional computational research has typically focused on isolated and/or subtotal systems to obtain partial information about the mechanism of the total system. The highly integrated computer resources of the post-K computer (supercomputer Fugaku) will be powerful enough to make such research obsolete; Fugaku will open frontiers to establish a new academic standard in computational chemistry and physics, and will facilitate understanding of complex phenomena in real materials and heterogeneous systems.

"The second collaborative symposium for experimental and industrial researchers" was held focusing on the theme of "Effective Use of Chemical Energy" in Sapporo on December 11th. Four researchers outside the project gave invited lectures. The fifth annual symposium of the project was also held in Sapporo on December 11th and 12th. During these symposia, more than 100 participants joined the discussions. We plan to maintain similar activities for the duration of the Flagship project.

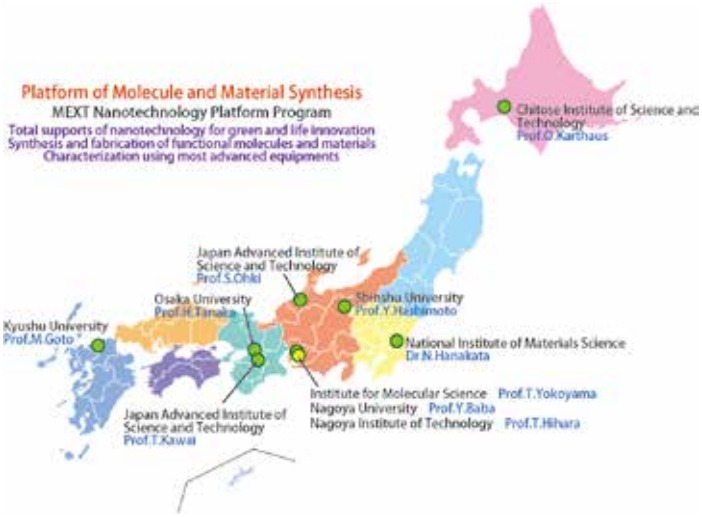


Left: Phase diagram of methane and ethane hydrates in temperature, pressure, and composition space, Right: Hydrate structure coexisting with liquid water.

(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 (MEXT) has been conducted in order to promote public usage of various nanotechnology facilities. This program will continue until March 2022 and consists of three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the management center of the platforms. Each platform consists of about ten organizations all over Japan. IMS conducts a representative core organization of the Molecule and Material Synthesis Platform. All the organizations in this platform are shown in Figure. In this platform, to promote green and life innovation

researches using nanotechnology related techniques not only for universities and government institutes but also for private companies, we will open various kinds of our facilities with total supports including molecular synthesis, materials fabrications, characterization, data analysis and scientific discussion. We will encourage applications not only to each element, but to combined usage of several supporting elements for bio-technology and green chemistry. In IMS, the number of accepted proposals in FY2018 amounted 158 (147 non-proprietary and 14 proprietary proposals, excluding inhouse applications from IMS) and the total number of days used for the supports is 3301 (2924 days for non-proprietary proposals and 98 days for proprietary ones).



List of Supports in IMS (FY2018)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, Y. Toyama, Y. Shibata
Organization Management in IMS			Y. Hyodo, Y. Funaki, M. Yokota
UVSOR Synchrotron Radiation	X-Ray Magnetic Circular Dichroism	T. Yokoyama	T. Koitaya
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Aoyama, N. Takada, T. Kondou
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Aoyama, T. Kondou, T. Toyota
Electron Microscopy	Field Emission Scanning Electron Microscopy	T. Yokoyama	Y. Matsuo
	Low vacuum Analytical Scanning Electron Microscopy		Y. Matsuo, M. Sakai
	Focus Ion Beam Processing		Y. Matsuo
X-rays	Single Crystal X-Ray Diffractometer		M. Fujiwara
	Low Temperature Single Crystal X-Ray Diffractometer for Microcrystals		Y. Okano
	Molecular Structure Analysis using Crystalline Sponge Method		K.Adachi
	Powder X-Ray Diffractometer		M. Fujiwara
	X-Ray Fluorescence Analysis		T. Ueda
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama
Electron Spectroscopy	Electron Spectroscopy for Chemical Analysis	T. Yokoyama	M. Sakai, S. Iki
	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	S. Kera, K. Tanaka	S. Ideta

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

(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 five-year project "Functioning of Inter-University Network for Efficient Utilization of Chemical Research Equipments" was launched. The network maintains an internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. 72 national universities as well as Institute for Molecular Science (total 73 organizations) all over Japan have been participating in the network. They are grouped into 12 local regions and in each region the regional committee discusses and determines the operation of regional network systems with the hub university chairing. There is no barrier for every user to access to any universities beyond his/her regional group. From 2009, the registered equipments are open to the researchers and students of all the public (prefectural *etc.*) and private universities. Since 2010, the project has been renamed "Inter-University Network for Common Utilization of Research Equipments" still keeping the original strategy and stable functioning. Last year we launched a new reservation and charging system that is more user-friendly, convenient and safe for a long period. The number of registered users amounts to 13,000 in 385 universities/institutions/companies covering over 3,500 laboratories in Japan (June, 2019). Usage of the network reaches almost 11,000 times per month and keeps growing in numbers. Moreover, we have actively provide various opportunities where technical staffs and users can improve their technical skills and frankly communicate with each other.

Okazaki Conference

(a) The 79th Okazaki Conference
Synthetic, Biological, and Hybrid Molecular Engines
(August 31–September 2, 2018)

Organizers: R. Iino (*IMS*), K. Kinbara (*Tokyo Tech*)

Invited Overseas Speaker: Z. Bryant (*Stanford Univ.*), O. Ces (*Imperial College London*), J. H. Choi (*Purdue Univ.*), P. Huang (*Stanford Univ.*), Y. Zhang (*Columbia Univ.*), G. Rapenne (*Nara Inst. Sci. Tech./Univ. Paul Sabatier, Toulouse*)

Synthetic and biological molecular machines have been extensively studied for a long time. However, these research fields have advanced independently, although both molecular machines have complementary advantages such as flexibility in molecular designs and highly specific advanced functions. Furthermore, there must be a common physical principle between synthetic and biological molecular machines. In the 79th Okazaki conference, we discussed how we can cooperate and merge these two highly relevant research fields toward the creation of "molecular engines," which efficiently and autonomously convert energy via mechanical motions.

(b) The 80th Okazaki Conference
Chirality-Induced Spin Selectivity and Its Related Phenomena
(May 15–18, 2019)

Organizers: H. Yamamoto (*IMS*), R. Naaman (*Weizmann Inst.*)

Invited Overseas Speaker: Ron Naaman (*Weizmann Inst.*), Helmut Zacharias (*Univ. Munster*), Ismael Diez Perez (*Kings College London*), Jie Song (*Shanghai Jiao Tong Univ.*), Jeanne Crassous (*Univ. Rennes 1*), Karl Heinz Ernst (*Empa*), Eric Vetter (*North Carolina State Univ.*), David Waldeck (*Univ. Pittsburgh*), Jean-Philippe Ansermet (*Ecole Polytechnique Federale Lausanne*), Michael Therien (*Duke Univ.*), Amnon Aharony (*Hebrew Univ.*), Ora Entin-Wohlman (*Ben Gurion Univ.*), Vladimiro Mujica (*Arizona State Univ.*), Xu Yang (*Univ. Groningen*), Ai-Min Guo (*Central South Univ.*), Yossi Paltiel (*Hebrew Univ.*), Sandipan Pramanik (*Univ. Alberta*), Claudio Fontanesi (*Univ. Studi Modena Reggio*), Narcis Avarvari (*Angers Univ.*), Jeremy Levy (*Univ. Pittsburgh*)

Recently, molecular chirality has been found to be effective at filtering an electron spin. This chirality-induced spin selectivity (CISS) is applicable to a wide range of science and technology including spintronics, electrochemistry, biochemistry, optical separation, and computational chemistry.

Exchange of the research achievements and ideas between researchers from different research fields is the aim of this conference, which should be fruitful for further development of this new field. We counted 62 participants at the conference, including 20 invited speakers from oversea countries. During the 80th Okazaki conference, participants have discussed how and why the CISS effect occurs in so diverse and different occasions, as well as its relationship towards related phenomena such as the Edelstein effect and magneto-chiral dichroism.

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) Molecular Simulation on Structural Change of Tritium-Substituted Polymeric Materials by Decay from Tritium to Helium-3

FUJIWARA, Susumu (*Kyoto Inst. Tech.*)
MIZUGUCHI, Tomoko (*Kyoto Inst. Tech.*)
SAKAI, Wataru (*Kyoto Inst. Tech.*)
LI, Haolun (*Kyoto Inst. Tech.*)
NAKAMURA, Hiroaki (*NIFS*)
HATANO, Yuji (*Univ. Toyama*)
SAITO, Seiki (*Yamagata Univ.*)
SAIKI, Toshiharu (*Keio Univ.*)
OTSUKA, Takao (*RIKEN*)
KENMOTSU, Takahiro (*Doshisha Univ.*)
ASO, Tsukasa (*Natl. Inst. Tech., Toyama College*)
YASUNAGA, Takuo (*Kyushu Inst. Tech.*)
OYA, Yasuhisa (*Shizuoka Univ.*)
TOGARI, Akihiro (*Shizuoka Univ.*)
WADA, Takuro (*Shizuoka Univ.*)
YONETANI, Yoshiaki (*QST*)
MIYANISHI, Hisanori *(Nagoya Univ.*)
SAITO, Shinji (*IMS*)

Tritium is radioactive hydrogen and is mostly produced by nuclear reaction from human activity. Tritium decays to helium-3 by beta decay with emissions of a beta-ray and an antineutrino with a half -life of 12.323 years. Since the range of beta rays emitted from tritium is short, external exposure is not problematic and protection against internal exposure is important. Beta rays may cause damage on macromolecules such as polymeric materials and DNA both directly and indirectly. Moreover, if substituted tritium in macromolecules decays to helium-3, their structure may be destabilized by chemical bond breakage, which is called decay effect. Although numerous experimental and computer simulation studies have been made on the damage of macromolecules through direct and indirect action, any studies have not been conducted on the damage of macromolecules through decay effect because of the difficulties in extracting the decay effect only.

In this project, we aim to predict the structural change of tritium-substituted macromolecules such as polymeric materials and DNA by a beta decay to helium-3 using molecular dynamics simulations.

Three meetings were held at IMS. Not only the core members (the applicants of this project) but also other related collaborators attended these meetings. The first two meetings were held to discuss the course of action for this project on June 6 and December 3, 2018. The third meeting was held to summarize the progress and discuss a future plan of this project on March 4–5, 2019.

(b) Construction of Synthetic Microdomains to Artificially Assemble Biological Polymers on Lipid Membranes Using Metal Complex Lipids

OHTANI, Ryo (*Kyushu Univ.*)
KAWANO, Kenichi (*Kyoto Univ.*)
KINOSHITA, Masanao (*Kyushu Univ.*)
YANAKA, Saeko (*IMS*)
KATO, Koichi (*IMS*)

Cell membranes are nonuniform entities characterized by heterogeneous molecular assemblies that mediate biological processes exemplified by signal transduction. Accumulating evidence has indicated that these microdomains comprise various lipid molecules including glycosphingolipids and cholesterol and serve as molecular platforms where specific biomolecules accumulate to perform sophisticated functions. To gain a deeper understanding of these complex membrane functions, we employed a multilateral approach in an attempt to artificially control membrane properties and their molecular assembly.

In this project, we created and applied *metal complex lipids* for (1) manipulating lipid membrane properties such as curvature and viscosity to construct synthetic domain architectures and (2) controlling assemblies of biological polymers thereon. The metal complex lipid consists of a metal complex moiety as its hydrophilic head and an alkyl chain as its hydrophobic tail. It exhibits different physical properties from those of natural lipid species, which further impacts lipid membrane properties. Through investigation of the influence of the metal complex lipids on phase-transition and molecular-assembling behaviors of both artificial and cell membranes, we successfully constructed an artificial phase separation system with micro-sized metal complex domains in living cell membranes. We intend to observe the metal complex domains using high-speed atomic force microscopy. Moreover, synthesis of new metal complex lipids hybridizable to biomolecules is also underway.

We held three collaboration meetings in the 2018 financial year to extensively discuss our research progress and future planning. The first and the third meetings were held at Yamate 3rd Bilding 2F small meeting room on May 12, 2018, and March 9, 2019, respectively. The second meeting was held at Kumamoto University on November 8, 2018, where RO was formerly posted.

(2) Research Symposia

(From Oct. 2018 to Sep. 2019)

Dates	Theme	Chair
Oct. 28, 2018	The 1st Hydride Ionics Seminar	**KOBAYASHI, Genki**
Nov. 30–Dec. 1, 2018	The International Symposium on Bioinorganic Chemistry 2018	**SHOJI, Osami** **AONO, Shigetoshi**
Jan. 15–16, 2019	Water at Interfaces 2018	**ONISHI, Hiroshi** **SUGIMOTO, Toshiki**
Mar. 3– 4, 2019	Coordination Chemistry for Controlling Hierarchical Structures and Functions	**UEMURA, Takashi** **MASAOKA, Shigeyuki**
Mar. 15–16, 2019	New Frontier in Protein Design & Engineering	**ARAI, Ryoichi** **KOGA, Nobuyasu**
May 21–22, 2019	Micro-Beam Analysis Workshop Atomic Level Imagings in Synchrotron-Radiation-Based Materials-Science Research	**MATSUI, Fumihiko**
May 28, 2019	The Challenge of Single Molecule Organic Chemistry	**NAKANISHI, Waka** **MOMIYAMA, Norie**
May 30, 2019	Fusion of Chemistry and Information Science —Toward New Innovative Chemistry—	**ADSCHIRI, Tadafumi** **YAMAMOTO, Hiroshi**
Jun. 10–11, 2019	Solid State Chemistry Forum	**KOBAYASHI, Genki**
Aug. 5– 6, 2019	Development of Novel Functional Molecular System Using Quantum Phase Degree of Freedom	**KAGAWA, Fumitaka** **YAMAMOTO, Hiroshi**
Aug. 8–10, 2019	Topological Physics and Organic Massless Dirac Systems	**TAJIMA, Naoya** **YOKOYAMA, Toshihiko** **NAKAMURA, Toshikazu**
Jun. 9, 2019	Meeting for Lectures at 59th Summer School on Molecular Science for Young Scientists	**KOMATSUBARA, Wataru** **SUGIMOTO, Toshiki**
May 15–18, 2019	Chirality-Induced Spin Selectivity and Its Related Phenomena	**YAMAMOTO, Hiroshi**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2018–Mar. 2019		Apr. 2019–Sep. 2019		Total		
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		2		1		3		3
Research Symposia		5		6		11		11
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		23	52	14	28	37	80	117
Use of Facility	Instrument Center		79		67		146	146
	Equipment Development Center	2	3	2	5	4	8	12
Use of UVSOR Facility		114	1	93	2	207	3	210
Use of Facility Program of the Computer Center						248*		248*

* from April 2018 to March 2019

Collaboration Programs

(1) International and Inter-Institutional Collaboration Symposia

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

Program	Coordinator	Date	Place
IMS-NCTU MOU Meeting	OKAMOTO, Hiromi (IMS) YAMAMOTO, Hiroshi (IMS) IINO, Ryota (IMS) FUJI, Takao (IMS)	2018.10.2–5	NCTU, Taiwan
The 2nd IMS-NANOTEC Joint Research Meeting	YAMAMOTO, Hiroshi (IMS) CHINSIRIKUL, Wannee (NANOTEC)	2018.11.22	IMS
SOKENDAI Asian Winter School "Challenges for New Frontiers in Molecular Science: From Basics to Advanced Researches"	NISHIMURA, Katsuyuki (IMS) KOBAYASHI, Genki (IMS)	2018.12.19	IMS
Workshop on NCTU-IMS Academic Cooperation 2019	IINO, Ryota (IMS)	2019.4.12	IMS
The 17th Japan-Korea Symposium on Molecular Science "Advances in Materials and Molecular Sciences"	KERA, Satoshi (IMS) ISHIZAKI, Akihito (IMS) KAWAI, Maki (IMS) KIM, Tae Kyu (Yonsei Univ.) LIM, Manho (Pusan Natl. Univ.)	2019.7.29–31	Nagoya, Japan

(2) IMS International Internship Program and SOKENDAI International Lecture & Training Courses

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	22*	–
SOKENDAI Asian Winter School (2018.12.19)	2	7†

* from Sep. 2018 to Aug. 2019, † include the IMS-IIP students

(3) IMS International Collaboration

Category	Number of People
International Joint Research Programs	61
International Use of Facilities Programs	41

from Sep. 2018 to Aug. 2019

(4) 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]	2006.12–2022.10	12	0
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2005. 1–2020. 2	0	0
Korea Advanced Institute of Science and Technology (KAIST) [Korea]	2008. 9–2020. 9	7	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2009.10–2019.10	9	1
Helmholtz Zentrum Berlin (HZB) [Germany]	2015. 1–2019. 6	1	0
Freie Universität Berlin (FUB) [Germany]	2013. 6–2022. 6	4	0
Indian Institute of Science Education and Research Kolkata (IISER Kolkata) [India]	2015.10–2019.10	1	0
Indian Institute of Science (IISc) [India]	2015.10–2019.10	0	1
National Nanotechnology Center, National Science and Technology Development Agency (NANOTEC/NSTDA) [Thailand]	2017.10–2022.10	8	1
Sungkyunkwan University (SKKU) [Korea]	2018. 4–2022. 3	0	0
University of Oulu [Finland]	2018. 5–2021. 5	4	0
National Chiao Tung University [Taiwan]	2018. 6–2023. 5	14	8
Peter Grünberg Institute, Forschungszentrum Jülich GmbH (FZJ) [Germany]	2018.10–2023. 9	2	3

from Sep. 2018 to Aug. 2019

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

Institution	Period	Accept	Send
Chulalongkorn University, Faculty of Science [Thailand]	2010. 4–2020. 3	4	1
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2021. 4	3	1
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2021. 7	2	1
Vidyasirimedhi Institute of Science and Technology [Thailand]	2018. 9–2023. 9	0	1

from Sep. 2018 to Aug. 2019