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 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

(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.

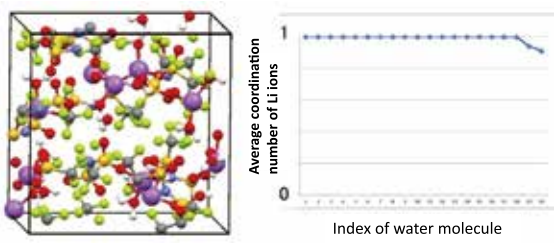
(a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT) Flagship Project, Priority Research Issue, "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use"

A new supercomputer, the so-called post-K computer, 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 46 institutions including 16 companies.

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 CO_2 and effective use of energies and resources produced by catalytic reactions. We will also collaborate with experimentalists in academia and researchers in industries to establish new energy technologies that 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 will be powerful enough to make such research obsolete; Post-K 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.

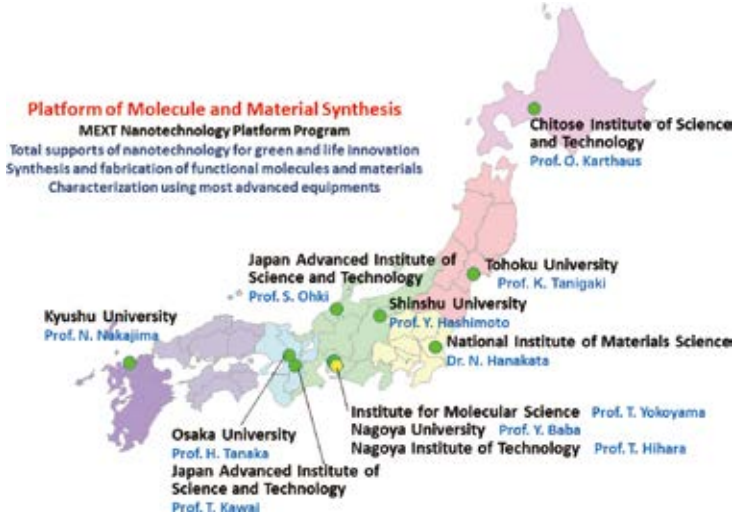
In the 2016 financial year, two symposia to promote collaboration with other national projects were held; *i.e.*, "The third symposium for collaboration of large experimental facilities and supercomputers" on September 1 2016, and "The first workshop for cooperation with the elements strategy initiative" on November 29 and 30. The third annual symposium of this project was also held on December 15 and 16, and more than 100 participants engaged in discussions. Furthermore, the research and development plan for the priority research issue "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use" was refined and submitted to MEXT. We plan to maintain similar activities for the duration of the Flagship project.



The mechanism of hydrate-melt electrolytes for high-energy-density aqueous batteries, was found computationally in this project. (Left) schematic picture of equilibrium state of newly-developed hydrate melt, (Right) coordination number of Li ions from each water molecule. *Nat. Energy* **1**, 16129 (2016).

(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 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 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 biotechnology and green chemistry. In IMS, the number of accepted proposals in FY2016 amounted 187 (161 non-proprietary and 25 proprietary proposals, excluding in-house applications from IMS) and the total number of days used for the supports is 3079 (2922 days for non-proprietary proposals and 147 days for proprietary ones).



List of Supports in IMS (FY2016)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, I. Noda, Y. Toyama, Y. Funaki, M. Yokota, N. Nakagawa, A. Ota, Y. Hyodo
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, Y. Uemura
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Suzui, M. Aoyama, N. Takada, T. Kondou, M. Nakano
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Suzui, M. Aoyama, H. Yoshida, T. Kondou, T. Toyota
Electron Microscopy	Field Emission Scanning Electron Microscopy	S. Kera	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
	Low Temperature Single Crystal X-Ray Diffractometer for Microcrystals		Y. Okano
	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	N. Kosugi	M. Sakai, Y. Inagaki
	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	N. Kosugi, S. Kera, K. Tanaka	H. Yamane, S. Ideta, T. Ueba
Electron Spin Resonance	Pulsed High Field ESR	T. Nakamura, S. Kera	M. Asada, S. Iki, M. Fujiwara
	X-Band CW ESR		S. Iki, M. Fujiwara
	X, Q-Band CW ESR		
SQUID	Superconducting Quantum Interference Device		S. Iki, M. Fujiwara
Thermal Analysis	Differential Scanning Calorimeter (Solutions)		S. Makita, H. Nagao
	Isothermal Titration Calorimeter (Solutions)		
	Calorimeter for solids		M. Fujiwara
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		S. Makita
Spectroscopy	Microscopic Raman Spectroscopy	S. Kera	M. Uruichi
	Fourier Transform Far Infrared Spectroscopy		
	Fluorescence Spectroscopy		T. Ueda
	Ultraviolet & Visible Absorption Spectroscopy		
	Circular Dichroism		S. Makita
Lasers	Picosecond Laser		T. Ueda
	Nanosecond Excimer/Dye Laser		T. Yamanaka
	Nanosecond Nd:YAG OPO Laser		
	Nanosecond Fluorinated Excimer Laser		
High Field NMR	920 MHz NMR Solutions & Solids	K. Kato, K. Nishimura S. Kera	S. Makita, H. Nagao
	800 MHz Solutions, Cryostat Probe	K. Kato	M. Yagi, S. Yanaka
	600 MHz Solids	K. Nishimura	
	600 MHz Solutions	S. Kera	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	
	Magnetic Thin Films	T. Yokoyama	Y. Takagi, 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 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. In July 2017, the number of registered users amounts to 11,500 in 251 universities/institutions/companies covering 2,788 laboratories in Japan. Usage of the network reaches almost 10,000 times per month and keeps growing in numbers. We are now reconstructing a new reservation and charging system that will be more user-friendly, convenient and safe for a long period. 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" was 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 76th Okazaki Conference
Advanced Spectroscopy of Organic Materials for Electronic Applications
(November 23–25, 2016)

Organizers: J. Schnadt (*Lund Univ., Sweden*), N. Koch (*Humboldt Univ. Berlin, Germany*), S. Sorensen (*Lund Univ., Sweden*), H. Yoshida (*Chiba Univ.*), H. Kondoh (*Keio Univ.*), J. Yoshinobu (*Univ. Tokyo*), N. Kosugi (*IMS*), S. Kera (*IMS*)

Invited Speakers: M. Zharnikov (*Heidelberg Univ., Germany*), O. L. A. Monti (*Univ. Arizona, U.S.A.*), S. Yamamoto (*Univ. Tokyo*), S. Kümmel (*Univ. Bayreuth, Germany*), A. Schöll (*Univ. Würzburg, Germany*), D. Lüftner (*Univ. Graz, Austria*), T. Fritz (*Univ. Jena, Germany*), H. Ishii (*Chiba Univ.*), Y. Nakayama (*TUS*), S. Duhm (*FUNSOM, China*), P. Krüger (*Chiba Univ.*), H. Peisert (*Univ. Tübingen, Germany*), H. Yoshida (*Chiba Univ.*), P. Amsalem (*Humboldt Univ. Berlin, Germany*), K. Akaike (*TUS*), J. Schnadt (*Lund Univ., Sweden*), L. Weinhardt (*KIT, Germany*), F. Gel'mukhanov (*KTH, Sweden*), M. Nagasaka (*IMS*), H. Kondoh (*Keio Univ.*), X. Liu (*Linköping Univ., Sweden*), N. Johansson (*Lund Univ., Sweden*), P. Shayesteh (*Lund Univ., Sweden*), Y. Takagi (*IMS*), T. Koitaya (*Univ. Tokyo*), M. Yoshida (*Keio Univ.*)

A rich of functionality found in the molecular-based materials has considerable attention in recent years. To improve the performance of the organic molecular devices and to realize any novel functional devices with molecules, deep insight into the electronic structure is requested. Moreover development in the experimental method and achievement in the novel technique as like in situ/operando techniques and time-resolved spectroscopy *etc.* is important to study. "Advanced Spectroscopy of Organic Materials for Electronic Applications" covers the topics related to spectroscopic techniques and theoretical modeling for the understanding the electronic structure of organic electronic materials and related interfaces. We counted 92 participants at the workshop, including 16 invited speakers from the oversea countries. We spent a lively and intimate atmosphere with participants to discuss the progress and development of a number of spectroscopy topics.

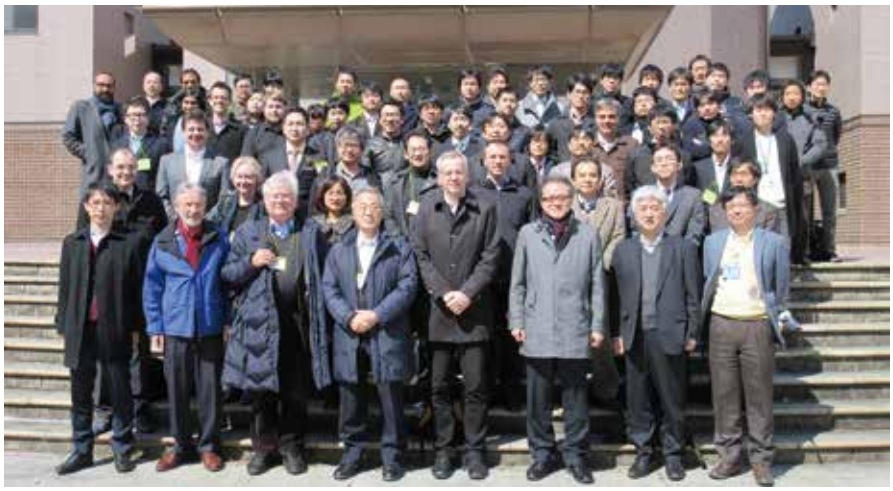
The 77th Okazaki Conference
International Symposium on Ultrafast Dynamics in Molecular and Material Sciences
(March 6–8, 2017)

Organizers: Y. Shigeta (*Univ. Tsukuba*), H. Ushiyama (*Univ. Tokyo*), T. Yamashita (*Univ. Tokyo*), S. Takahashi (*Univ. Tokyo*), M. Fujii (*Univ. Tokyo*) , S. Saito (*IMS*)

Invited Speakers: W. Domcke (*Tech. Univ. München, Germany*), T. Suzuki (*Kyoto Univ.*), K. Takatsuka (*Kyoto Univ.*), I. Barth (*Max Planck Inst., Germany*), T. Brixner (*Univ. Würzburg, Germany*), I. Burghardt (*Goethe Univ. Frankfurt, Germany*), O. Kühn (*Univ. Rostock, Germany*), N. T. Maitra (*City Univ. New York, U.S.A.*), I. Manz (*Freie Univ. Berlin & Shanxi Univ.*), T. F. Miller III (*Caltech, U.S.A.*), O.V. Prezhdo (*California Southern Univ., U.S.A.*), H. Wörner (*ETH, Switzerland*), S. Adachi (*KEK*), H. Benten (*NAIST*), T. Fujisawa (*Saga Univ.*), M. Fushitani (*Nagoya Univ.*), M. Hada (*Okayama Univ.*), Y. Harabuchi (*Hokkaido Univ.*), M. Kanno (*Tohoku Univ.*), R. Kanya (*Univ. Tokyo*), H.-D. Kim (*Kyoto Univ.*), T. Otobe (*QST*), T. Sato (*Univ. Tokyo*), M. Shibuta (*Keio Univ.*), T. Takaya (*Gakushuin Univ.*), T. Yasuike (*Open Air Univ.*)

Considering chemical reactions, one always adopts the Born-Oppenheimer approximation, where electronic and nuclear degrees of freedom are separately treated. However, with recent progresses in the experimental technology for the

ultrafast spectroscopy, highly accurate observations on nuclear dynamics and electron dynamics in molecules are available to analyze the ultrafast phenomena in molecules and materials. This workshop focused on theoretical and experimental studies on ultrafast (atto to femto second) dynamics of molecules and materials and was organized into 3 days symposia with a poster session that are designed to highlight many of the cutting edge developments in this field.

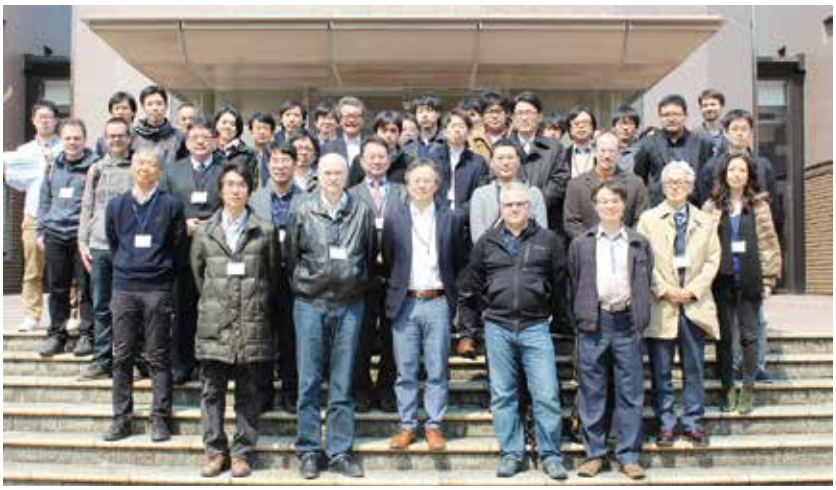


The 78th Okazaki Conference
Grand Challenges in Small-Angle Scattering
(March 18–20, 2017)

Organizers: S. Akiyama (*IMS*), H. Kamikubo (*NAIST*), M. Sugiyama (*Kyoto Univ.*)

Invited Speakers: D. Svergun (*EMBL Hamburg, Germany*), H. Kamikubo (*NAIST*), P. Bernado (*Cent. Biochimie Structurale, France*), N. Ando (*Princeton Univ., U.S.A.*), U.-S. Jeng (*NSRRC, Taiwan*), S. Lee (*Sungkyunkwan Univ., Korea*), S. Akiyama (*IMS*), M. Sugiyama (*Kyoto Univ.*), F. Gabel (*IBS, Grenoble, France*), S. Fujiwara (*QST*), R. Biehl (*JCNS, Julich, Germany*), K. Ito (*Rigaku Corp.*), R. Arai (*Shinshu Univ.*), S. Toma-Fukai (*Univ. Tokyo*), M. Petoukhov (*Russian Acad. Sci, Russia*), T. Oroguchi (*Keio Univ.*), J. Hub (*Inst. Microbiology Genetics, Germany*)

Small-angle scattering is one of the effective analytical tools for hierarchical bio-molecular systems, providing size and shape information from sub-nanometer to micrometer in real-time. In this conference, the fundamentals of the solution scattering will be first overviewed, and then recent applications of x-ray/neutron solution scattering to the molecular system sciences will be shared with life-science students/researchers in mind. Furthermore, the organizers would like to provide an opportunity to think about an East Asian SAS community through discussions with the leading scientists invited from Taiwan and Korea SAS communities.



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. Frontier of the Research on Biological Trace Elements

ITOH, Shinobu (*Osaka Univ.*)
KANO, Kenji (*Kyoto Univ.*)
HIROTA, Shun (*NAIST*)
SHIRO, Yoshitsugu (*Univ. Hyogo*)
AONO, Shigetoshi (*IMS*)

A variety of essential trace elements including transition metal ions are required for normal biological functions. Though they are essential for biological functions, their intracellular concentrations have to control very strictly to maintain cellular homeostasis. Once the homeostasis is disrupted, deficit or excess of specific metal ions is induced to lead diseases. Transition metal ions such as iron, copper, cobalt, nickel, molybdenum, and zinc are utilized as the active sites and/or components of prosthetic groups in metalloproteins, which play crucial roles for transport and activation of small molecules, electron transfer, redox catalysis, and signal transduction. Recently, progress in experimental methods for structural and spectroscopic analyses makes detail studies on the metabolism, functions, and regulation of these trace metal ions in biological systems possible at the molecular level. In this project, we aimed for understanding the functional roles and the regulatory mechanisms of these trace metal ions in biological systems, based on which we will develop the basic research on biomolecular science, which can be contributed for industrial and medical applications. The feasibility studies on the following topics were carried out in this project for the preparation of a grant application to Grant-in-Aid for Scientific Research on Innovative Areas.

1. Elucidation of structure and function of metalloproteins

In this project, we have studied and searched new research targets on the structural and functional elucidation of metalloproteins and metalloenzymes that are responsible for the activation or binding/transport of small molecules, energy transfer/metabolism, and signal transduction.

2. Industrial application of metalloproteins

The feasibility of industrial application of metalloproteins and metalloenzymes have been studied and searched for developing catalysts, fuel cells, sensors, biocompatible materials, and tailor-made artificial metalloenzymes.

3. Medical application of metalloproteins

The feasibility of industrial application of metalloproteins and metalloenzymes have been studied and searched for elucidating the molecular mechanisms of the homeostasis for essential trace elements, of metal-transport and signal transduction reactions, and of protein–protein interactions regulating biological functions.

Two meetings only the core members (the applicants of this project) attended were held to discuss course of action for this project on April 1–2, and April 30, 2016. The third meeting was held at Okazaki Conference Center on May 22, 2016, where 14 speakers including the core members presented their research topics and discussed the feasibility of this project. The fourth meeting was held at IMS room 302 on March 30–31, 2017, where 13 speakers presented their research topics and discussed a future plan to apply the grant.

B. Vibrational Spectroscopy by Quantum Technology

SHIKANO, Yutaka (*IMS*)
NAKAMURA, Kazutaka (*Tokyo Tech*)
KAYANUMA, Yosuke (*Tokyo Tech*)
HORIKIRI, Tomoyuki (*Yokohama Natl. Univ.*)
KOBAYASHI, Hirokazu (*Kochi Univ. Tech.*)
UEDA, Tadashi (*IMS*)
OKANO, Yasuaki (*IMS*)

In order to build up the optical spectroscopy technique by the help of quantum technology, we developed theory of quantum measurement theory and constructed the spectroscopy setups for joint study on the pump-probe experiment under the wide wavelength picosecond laser system and the fixed wavelength (near 800 nm) femtosecond laser system in IMS. Also, in Tokyo Tech, we took the vibrational spectroscopy for the condensed phase system and measured the coherent phonon properties of semiconductor and diamond. We successfully demonstrated the coherent control a la the gas phase experiment and also the long-time lifetime measurement to show the spectral diffusion in terms of molecular science. Furthermore, we will plan to catch up how to emerge the coherence of phonon; the stimulated emission by phonon or other mechanism.

References

1) M. Tukiainen, H. Kobayashi and Y. Shikano, *Phys. Rev. A* **95**, 052301 (6 pages) (2017).
2) Y. Shikano, *AIP Conf. Proc.* **1871**, 020001 (7 pages) (2017).

(2) Research Symposia

(From Oct. 2016 to Sep. 2017)

Dates	Theme	Chair
Nov. 10–11, 2016	Development and Perspective for Next Generation of Molecular Catalyst	**MOMIYAMA, Norie**
Dec. 2, 2016	Frontiers in Surface Science Techniques and Molecular Science (7^{th} Workshop for Young Researchers in Vacuum and Surface Sciences)	**UEBA, Takahiro** **KERA, Satoshi**
Dec. 7– 8, 2016	Advanced Electron Spin Measurement to Investigate for the Origin of Biological and Material Functions	**KOBORI, Yasuhiro** **NAKAMURA, Toshikazu**
Mar. 6– 7, 2017	Information Control and Function Interlock Based on Metal Complexes	**OHBA, Masaaki** **MASAOKA, Shigeyuki**
Jun. 12, 2017	Frontier of Local Structural and Functional Analysis of Liquid Water	**TAKAHARA, Atsushi** **KOSUGI, Nobuhiro**
Jun. 14, 2017	Molecular Scinece of Enzymatic Catalysis	**KONNO, Michiko** **MASAOKA, Shigeyuki**
Jun. 24–25, 2017	Japan-China Joint Interdisciplinary Symposium on Coodination-Based Hybrid Materials	**IMAOKA, Takane** **MASAOKA, Shigeyuki**
Jul. 17–18, 2017	Heterogeneous Fluctuations in Science: The Nishikawa Line —The Second Critical Point	**ABE, Hiroshi** **KERA, Satoshi**
Aug. 18–19, 2017	Mechanical Interactions between Molecules and Radiation Fields under Resonance: Toward Molecular Level Manipulation	**HOSOKAWA, Chie** **OKAMOTO, Hiromi**
Aug. 26–27, 2017	Biometals Dynamics Meeting	**SHIRO, Yoshitsugu** **AONO, Shigetoshi**
Jun. 18, 2017	Meeting for Lectures at 57^{th} Summer School on Molecular Science for Young Scientists	**OKINO, Shunnosuke** **FURUTANI, Yuji**
Jul. 6– 7, 2017	The 15^{th} ESR Summer School: Principle and Perspective of Multi-Frequency Pulsed ESR Measurements	**EMA, Fumitoshi** **NAKAMURA, Toshikazu**
Nov. 23–25, 2016	Advanced Spectroscopy of Organic Materials for Electronic Applications	**KERA, Satoshi**
Mar. 6– 8, 2017	International Symposium on Ultrafast Dynamics in Molecular and Material Sciences	**SHIGETA, Yasuteru** **SAITO, Shinji**
Mar. 18–20, 2017	Grand Challenges in Small-Angle Scattering	**AKIYAMA, Shuji**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2016–Mar. 2017		Apr. 2017–Sep. 2017		Total		
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		0		1		1		1
Research Symposia		4		6		10		10
Research Symposia for Young Researchers		0		2		2		2
Cooperative Research		45	28	35	33	80	61	141
Use of Facility	Instrument Center		72		71		143	143
	Equipment Development Center	1	2	1	2	2	4	6
Use of UVSOR Facility		77	17	53	20	130	37	167
Use of Facility Program of the Computer Center						221*		221*

* from April 2016 to March 2017

Collaboration Programs

(a) 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 Asian International Symposium "Japan-Korea-Taiwan Bioinorganic Chemistry Symposium"	AONO, Shigetoshi (IMS)	2016.9.29–9.30	IMS
The 9th Korea-Japan Seminars on Biomolecular Sciences: Experiments and Simulations	AONO, Shigetoshi (IMS) KATO, Koichi (IMS) LEE, Jooyoung (KIAS)	2016.11.13–11.16	Commodore Hotel, Gyeongju, Korea
The 76th Okazaki Conference "Advanced Spectroscopy of Organic Materials for Electronic Applications"	KERA, Satoshi (IMS) SCHNADT, Joachim (Lund Univ., Sweden) KOCH, Norbert (Humboldt Univ. Berlin, Germany) SORENSEN, Stacey (Lund Univ., Sweden) YOSHIDA, Hiroyuki (Chiba Univ) KONDOH, Hiroshi (Keio Univ) YOSHINOBU, Jun (Univ. Tokyo) KOSUGI, Nobuhiro (IMS)	2016.11.23–11.25	IMS
SOKENDAI Asian Winter School "Challenges for New Frontiers in Molecular Science: From Basics to Advanced Researches"	MOMIYAMA, Norie (IMS) KOGA, Nobuyasu (IMS)	2016.12.14–12.15	IMS
The 3rd China-Japan-Korea Workshop on Theoretical and Computational Chemistry (CJK-WTCC-III)	JUNG, Yousung (KAIST) KIM, Woo Youn (KAIST) YEOM, Min Sun (KISTI)	2017.1.10–1.13	KAIST, Daejeon, Korea
The 77th Okazaki Conference "International Symposium on Ultrafast Dynamics in Molecular and Material Sciences"	SAITO, Shinji (IMS) SHIGETA, Yasuteru (Univ. Tsukuba) USHIYAMA, Hiroshi (Univ. Tokyo) YAMASHITA, Takefumi (Univ. Tokyo) TAKAHASHI, Satoshi (Univ. Tokyo) FUJII, Mikiya (Univ. Tokyo)	2017.3.6–3.8	IMS
The 78th Okazaki Conference "Grand Challenges in Small-Angle Scattering"	AKIYAMA, Shuji (IMS) KAMIKUBO, Hironari (NAIST) SUGIYAMA, Masaaki (Kyoto Univ.)	2017.3.18–3.20	IMS
2017 Korea-Japan Molecular Science Symposium "Frontiers in Molecular Science: Structure, Dynamics, and Function of Molecules and Complexes"	JOO, Taiha (POSTECH) KAWAI, Maki (IMS) RYU, Sunmin (POSTECH) KIM, Tae Kyu (PNU) KERA, Satoshi (IMS) SAITO, Shinji (IMS)	2017.7.10–7.12	Haeundae Tivoli Hotel, Busan, Korea

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

Category	Number of People	
	Overseas	Domestic
IMS International Internship Program (IMS-IIP)	24*	–
SOKENDAI Asian Winter School (2016.12.14–12.15)	7†	5

* from Sep. 2016 to Aug. 2017, † include the IMS-IIP students

(c) IMS International Collaboration

Category	Number of People
International Joint Research Programs	63
International Use of Facilities Programs	40

from Sep. 2016 to Aug. 2017

(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]	2014.11–2018.11	0	0
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2017. 2–2020. 2	1	0
Institute of Chemistry, Chinese Academy of Science (ICCAS) [China]	2013. 9–2018. 9	1	0
Korea Advanced Institute of Science and Technology (KAIST) [Korea]	2016. 9–2020. 9	0	2
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2014.10–2019.10	7	3
Helmholtz Zentrum Berlin (HZB) [Germany] Freie Universität Berlin (FUB) [Germany]	2016. 6–2019. 6	7	2
Indian Institute of Science Education and Research Kolkata (IISER Kolkata) [India]	2015.10–2019.10	2	0
Indian Institute of Science (IISc) [India]	2015.10–2019.10	0	0

from Sep. 2016 to Aug. 2017

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

Institution	Period	Accept	Send
Chulalongkorn University, Faculty of Science [Thailand]	2010. 4–2020. 3	5	3
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2021. 4	3	6
Mahidol University, Faculty of Science [Thailand]	2014. 3–2019. 3	4	1
Nanyang Technological University, College of Science [Singapore]	2014. 3–2019. 3	0	0
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2019. 3	0	0

from Sep. 2016 to Aug. 2017