Special Research Projects

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

- (a) The Ministry of Education, Culture, Sports, Science and Technology HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)" Field 2 "New Materials and Energy Creation"
- "Construction of Innovative High Performance Computing Infrastructure (HPCI)"
 (b) The Ministry of Education, Culture, Sports, Science and Technology (MEXT)
 Flagship 2020 Project, Priority Research 5
 - "Development of New Fundamental Technologies for High Efficiency Energy Creation, Conversion/Storage, and Use"
- (c) MEXT Nanotechnology Platform Program Platform of Molecule and Material Synthesis
- (d) Inter-University Network for Efficient Utilization of Research Equipments
- (e) Consortium for Photon Science and Technology (C-PhoST)

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) The Ministry of Education, Culture, Sports, Science and Technology HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)" Field 2 "New Materials and Energy Creation" "Construction of Innovative High Performance Computing Infrastructure (HPCI)"

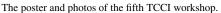
HPCI strategy programs "SPIRE" aims at promoting scientific research activities using "K-computer" at RIKEN Advanced Institute for Computational Science. In the strategic filed 2 of SPIRE, the Institute for Solid State Physics (ISSP) of the University of Tokyo, Institute for Molecular Science (IMS), and Institute for Material Research (IMR) of Tohoku University have been selected as the members of a strategic organization. The project started in September 2010 for "Computational Material Science: Turning the Headwaters of Basic Science into a Torrent of Innovations in Functional Materials and Energy Conversion" as its main strategic target. To promote the activities of the strategic organizations, a new community "Computational Materials Science Initiative (CMSI)" consisting of research fields of condensed matter physics, molecular science and materials science was launched.

Theoretical and Computational Chemistry Initiative (TCCI)

at IMS completed the activities of the 2014 academic year: (1) TCCI organized the fifth TCCI workshop including invited talks of several experimental chemists, and the other one for industry-academic partnership, (2)TCCI also sponsored the eighteenth summer school of Molecular Simulations, two TCCI winter colleges (molecular simulations, and quantum chemistry), and one workshop for massively parallel programming, (3)Research Center for Computational Science (RCCS) continued to provide a part of its computing resources to the SPIRE project as one of the activities of TCCI, and (5) TCCI assisted to form a new group for the Post-K computer project.

The 2015 academic year is the last year for TCCI. TCCI is going to complete the activities above and promote the research using K-computer and the computational molecular science field, as much as possible.













(b) The Ministry of Education, Culture, Sports, Science and Technology (MEXT) Flagship 2020 Project, Priority Research 5 "Development of New Fundamental Technologies for High Efficiency 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 High Efficiency 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.

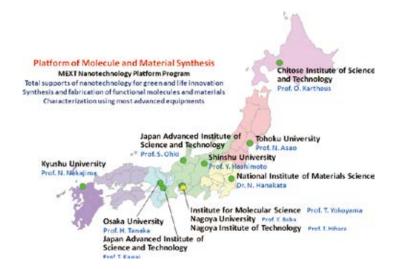
We propose to perform these state-of-the-art calculations to unravel the following issues; Branch A: Production and storage of alternative energy sources with solar cells and artificial photosynthesis; Branch B: Conversion and storage of energies produced in fuel cells and rechargeable batteries; Branch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

(c) 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 FY2014 amounted 169 (147 non-proprietary and 22 proprietary proposals, excluding applications from IMS) and the total number of days used for the supports is 2693 (2627 days for non-proprietary proposals and 66 days for proprietary ones).



List of Supports in IMS (FY2015)

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		Inorganic Materials	G. Kobayashi	

(d) Inter-University Network for Efficient Utilization of Research Equipments

It is highly important to improve the supporting environment for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting research and education in high standard. To install such sophisticated instruments, tremendous amount of budgets would be necessary. In 2007, for constructing a national-wide network to provide the easy access 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 to 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 universities. Since 2010, the project name has been renamed "Inter-University Network for Efficient Utilization of Research Equipments," still keeping the original strategy and stable functioning. In March 2015, the number of user registrants amounts to 10,293 in 170 universities/institutions/companies covering 2,486 laboratories in Japan. Usage of the network reaches almost 10,000 times per month and keeps growing in numbers.

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

In order to establish strong bases in the research and education in optical science, a new 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), JAEA (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, semiconductor lasers, and coherent control. Emphasis is placed in the education of young researchers to be capable of taking leaderships in scientific projects through participation in the forefront researches taking place at C-PhoST and in international collaborations.

Okazaki Conference

The 74th Okazaki Conference Frontier of X-Ray Absorption Spectroscopy and Molecular Science (February 3–5, 2015)

Organizers: T. Yokoyama (*IMS*), K. Asakura (*Hokkaido Univ*.)

Invited Oversea Lecturers: T. -K. Sham (*Univ. West. Ontario*), A. Rogalev (*ESRF*), P. Fischer (*LBNL & UC Santa Cruz*), L. X. Chen (*ANL & Northwestern Univ.*), S. P. Cramer (*UC Davis & ALS*)

Invited Oversea Lecturers: S. Takakusagi (Hokkaido Univ.), T. Miyanaga (Hirosaki Univ.), H. Oyanagi (AIST), H. Abe (KEK-PF), S. Adachi (KEK-PF), T. Masuda (NIMS), Y. Takahashi (Univ. Tokyo), M. Uo (Tokyo Med. Dent. Univ.), M. Tada (Nagoya Univ.), T. Katayama (JASRI/SPring-8), T. Uruga (JASRI/SPring-8), N. Ishimatsu (Hiroshima Univ.), T. Ohigashi (IMS), M. Nagasaka (IMS), Y. Takagi (IMS), Y. Uemura (IMS)

The 74th Okazaki Conference, designated as "Frontier of X-ray Absorption Spectroscopy and Molecular Science" was held on February 3–5, 2015 at the Okazaki Conference Center.

Following the celebrated tradition of the preceding Okazaki Conferences, of which origin dated back to just after the foundation of IMS, the conference focused on the topic that is emerging as a fundamental issue in the field of molecular science and related research area. This time, 21 invited lectures including five oversea lecturers represented cutting-edge researches, and the number of participants was 50. We have discussed about new science that can be opened by advanced XAFS (X-ray Absorption Fine Structure) techniques like spatial and/or time-resolved measurements. Although XAFS has matured as a sophisticated promising technique, recent progress based on the advance of synchrotron radiation light sources is found to be really outstanding. We have summarized the advanced XAFS methods and discuss near-future XAFS techniques and more importantly new science. It was quite fruitful since the new XAFS science discussed could contribute to construction plans of diffraction-limited synchrotron radiation facilities in Japan.



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. Novel Power Generation System with a Power Delivery Integrated Circuits, suitable for Energy Harvesting

MIYAMOTO, Jun-ichi (*Chubu Univ.*) HIRAMOTO, Masahiro (*IMS*) KAJI, Toshihiko (*IMS*) SATO, Motoyasu (*Chubu Univ.*) ITOH, Hibiki (*Chubu Univ.*) KATO, Akira (*Chubu Univ.*)

Recently, energy harvesting technology has been intensively investigated not only for saving natural resources but for applying to sensors or mobile devices.¹⁾ The project is proposing a novel power generation system suitable for energy harvesting. Generally, natural power sources are spread over the world, but they are thin and are unstable, influenced by the circumstances. Moreover, the generated voltage by conversion devices is low (< 1.0). So, it is difficult to use conventional power generation system, applied to Silicon based Solar Cells. Now, we developed a dedicated device, named Power Delivery Integrated Circuits (PDIC)²⁾ in order to collect the electric power effectively, and propose a novel power generation system. For the verification of its effectiveness, we carried out a field test, utilizing a Dye Sensitized Solar Cell (DSSC) as an energy conversion device, since it is applicable to symbiotic power generation system with plants.

Concept of proposed power generation system is shown in Figure 1. The bunch of DSSCs is connected in parallel to the PDIC. The summation of electric power is outputted in "PW_SUM" terminal. Since inactive DSSCs, which are determined by the comparison data of generated voltage with the reference voltage "VREF," are disconnected from the system, no leakage current flows toward inactive DSSCs. By using transfergates, there is little voltage loss between DSSCs and PW_SUM. For actual use, a DC-to-DC converter is connected to the driven load, if necessary.

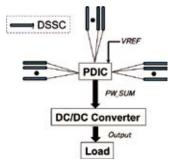


Figure 1. Concept of Novel Power Generation System.

The field test photo is shown in Figure 2. A hand-made DSSC consists of TiO₂ film deposited on FTO, together with dye and electrolyte. The counter electrode is made of platinum film. Electric contact between the TiO₂ particles was produced by sintering with sophisticated temperature ramping sequence. In this Figure, 16 DSSCs are connected to the PDIC.



Figure 2. Field Test Photo.

Figure 3 shows the PW_SUM voltage wave form with 100Ω resister load. In the Figure, at first, the PDIC disconnects all the DSSCs from the system. Within this reset and monitoring period, PW_SUM naturally stays low. Next, these DSSCs are connected one by one to the system. As High "Dout" means the DSSC is active, the Figure shows all of the 16 DSSCs are active. If the load impedance of PW_SUM is high enough, the voltage reaches inherent voltage rapidly, but if the impedance is low, the wave form looks like stairs as shown in the Figure. So, the PDIC, accumulating the power of DSSCs, works properly as designed. Since the PDIC was designed, and was fabricated with the 0.18µm CMOS, no DC current flows except for the voltage monitoring period. Note that it is easy to save PDIC power consumption negligibly small in comparison with the generated power, because the circumstance of the system changes gradually and the monitoring period can be set as long enough.

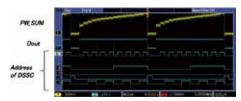


Figure 3. PW_SUM wave form with 100Ω load.

Currently, the characteristics of DSSC are sensitive to fabrication process parameters. The variation is detected by the PDIC. Figure 4 shows open-circuit-voltage variation of 16DSSCs, which is monitored by changing VREF. If VREF is

500 mV, all the DSSCs are active. But, if VREF is raised to 600 mV, 10 out of 16 DSSCs go inactive. Thanks to the parallel connection, a few failure DSSCs give little affection to the whole system performance. But, as the location of an inactive DSSC is easily identified, it can be replaced, if necessary.

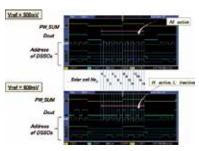


Figure 4. Dout dependence on VREF. Active or inactive states of individual DSSCs are shown.

By the field test, using DSSCs, proposed power generation system is demonstrated to work well. The future work is to improve the performance and to add some functions to the PDIC by feed-backing the data of field tests.

Acknowledgement

This work is supported by VDEC (VLSI Design and Education Center), the University of Tokyo in collaboration with Cadence Design Systems, Inc.

References

- 1) http://paulinevandongen.nl/projects/wearable-solar-shirt/
- J. Miyamoto, M. Hiramoto, T. Kaji, M. Sato, H. Itoh and A. Kato, "Development of a Power Delivery IC for Wavelength Selective Solar Cells," Institutes for Molecular Science, *Annual Review 2014*, p. 114 (2015).

(2) Research Symposia

(From Oct. 2014 to Sep. 2015)

Dates	Theme	(From Oct. 2014 to Sep. 2015) Chair
Nov. 21–22, 2014	Workshop on Next-Generation Synchrotron Light Sources —Towards a Road-Map of Synchrotron Light Sources in Japan beyond 3 rd Generation Sources and SASE-FEL	KATOH, Masahiro
Dec. 20, 2014	Solution Scattering as Research Tools of Molecular Systems	AKIYAMA, Shuji
Jan. 6– 7, 2015	Frontier of Bioinorganic Chemistry and Future Prospect: Elucidation of Functional Mechanisms of Metal Ions and Biomolecules, Their Modeling and Application	HAYASHI, Takashi AONO, Shigetoshi
Feb. 21–23, 2015	Workshop on Hierarchy of Quantum Mechanics	SHIKANO, Yutaka
Mar. 15–16, 2015	Construction and Function of Superstructure Compounds Containing Metal Ions—The Current Situation and Future Prospects of Interdisciplinary Fields of Coordination Chemistry	NIHEI, Masayuki MURAHASHI, Tetsuro
Apr. 20–21, 2015	Thinking of Proton Permeation inside Membrane Protein	KANDORI, Hideki IINO, Ryota
Jun. 12–13, 2015	Supramolecular Dynamics at the Interface of Chemistry and Biology	UENO, Takafumi IINO, Ryota
Jun. 27–28, 2015	Meeting on Chiral Magnetism and Optical Properties	INOUE, Katsuya OKAMOTO, Hiromi
Sep. 7– 8, 2015	Future Perspectives of Soft X-Ray Imaging	OHIGASHI, Takuji
Jun. 27, 2015	Preparation Meeting for 55 th Young Researchers Society for Molecular Science, 2015 Summer School	TANAKA, Shunsuke FURUTANI, Yuji

(3) Numbers of Joint Studies Programs

Categories		Oct. 2014-	-Mar. 2015	Apr. 2015	–Sep. 2015		Total	
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		0		2		2		2
Research Symposia		5		4		9		9
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		35	31	33	35	68	66	134
	Instrument Center	20	61	7	46	27	107	134
Use of Facility	Equipment Development Center	6	4	4	5	10	9	19
Use of UVSOR Facility		63	24	57	16	120	40	160
Use of Facility Program of the Computer Center						199*		199*

^{*} from April 2014 to March 2015

Collaboration Programs

(a) International Inter-Institutional Collaboration Symposia

Several international symposia and workshops in molecular science are held in IMS. Some workshops for international

collaboration are organized with our MOU partners in the MOU partner's country as well as in Japan:

Program	Coordinator	Date	Place
The 7 th Korea-Japan Seminar on Biomolecular Sciences: Experiments and Simulations	AONO, Shigetoshi (IMS) KATO, Koichi (IMS) KUWAJIMA, Kunihiro (Sokendai/KIAS) LEE, Jooyoung (KIAS)	2014.11.26–11.28	KIAS, Seoul, Korea
The Winter School of SOKENDAI/Asian CORE Program "Research and Its Challenges in Molecular Science: Fundamentals and State-of-the-Art"	YANAI, Takeshi (IMS) YAMAMOTO, Hiroshi (IMS) AKIYAMA, Shuji (IMS) UOZUMI, Yasuhiro (IMS) KIM, Bongsoo (KAIST, Korea) GE, Maofa (CAS, China) CHEN, Kuei-Hsien (IAMS, Taiwan)	2015.1.13–1.16	IMS
CU-IMS Joint Workshop	WACHARASINDHU, Sumrit (CU, Thailand)	2015.1.23–1.24	Chulalongkorn University, Bangkok, Thailand
Okazaki Conference "Frontier of X-Ray Absorption Spectroscopy and Molecular Science"	YOKOYAMA, Toshihiko (IMS)	2015.2.3–2.5	IMS
JSPS-DST Asian Academic Seminar: Structure, Dynamics, and Functionality of Molecules and Materials	OHMINE, Iwao (IMS) ENOKI, Toshiaki (TIT) IWASAWA, Yasuhiro (UEC) KOSHIHARA, Shin-ya (TIT) SAITO, Shinji (IMS) YAMAMOTO, Hiroshi (IMS) MUKHERJEE, Rabi N. (IISER, India) SANYAL, Milan K. (SINP, India) BATTACHARYYA, Kankan (IACS, India)	2015.3.6–3.10	Indian Association for the Cultivation of Science (IACS), Indian Institute of Science Education and Research (IISER), Kolkata, India
Workshop on Soft X-Ray in Energy and Time (SXET)	AZIZ, Emad Flear (HZB,) KOSUGI, Nobuhiro (IMS) CRAMER, Stephen P. (LBNL) GESSNER, Oliver (LBNL)	2015.8.20–8.21	Helmholtz Zentrum Berlin (HZB), Germany

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

Category	Number of People		
	Overseas	Domestic	
IMS International Internship Program	19*	-	
SOKENDAI Asian Winter School (2015.1.13–1.16) (Co-hosted with Asian CORE Program)	51	42	

^{*} from Sep. 2014 to Aug. 2015

(c) IMS International Collaboration

Category	Number of People
International Joint Research Programs	50
International Use of Facilities Programs	43

^{*} from Sep. 2014 to Aug. 2015

(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	11
Institute of Atomic and Molecular Sciences (IAMS) [Taiwan]	2014. 2–2017. 2	15	0
Institute of Chemistry Chinese Academy of Science (ICCAS) [China]	2013. 9–2018. 9	15	0
Korea Advanced Institute of Science and Technology (KAIST) [Korea]	2012. 9–2016. 9	11	0
École Nationale Supérieure de Chimie de Paris (ENSCP) [France]	2014.10-2019.10	6	1
Indian Association for the Cultivation of Science (IACS) [India]	2013. 3–2017. 3	10	7
Freie Universität Berlin (FUB) [Germany]	2013. 6–2016. 6	10	0
Helmholtz Zentrum Berlin (HZB) [Germany]	2015. 1–2016. 6	6	5

^{*} from Sep. 2014 to Aug. 2015

 $A cademic\ Exchange\ Agreement\ with\ Overseas\ Universities/Institutes\ (SOKENDAI)\ as\ follows\ ;$

Institution	Period	Accept	Send
Chulalongkorn University, Faculty of Science [Thailand]	2010. 4–2018. 3	5	5
Kasetsart University, Faculty of Science [Thailand]	2011. 3–2016. 3	9	0
Mahidol University, Faculty of Science [Thailand]	2014. 3–2019. 3	1	0
Nanyang Technological University, College of Science [Singapore]	2014. 3–2019. 3	1	0
University of Malaya, Faculty of Science [Malaysia]	2014. 3–2019. 3	3	0

^{*} from Sep. 2014 to Aug. 2015