Advisory Report

December 2019

Institute for Molecular Science
Advisory Council

Preface

The Advisory Council of the Institute for Molecular Science (IMSAC) convened from December 9th to 11th 2019 at IMS in Okazaki.

At the opening presentation, Maki Kawai, Director General of IMS, outlined the mission of the institute and her operation of the institute during the period from April 2016 to the present. In addition, she provided the following Terms of References as guidelines for the IMSAC to provide advice and recommendations.

The IMSAC is asked to advise on the governance, strategies, research systems, and management policies necessary for IMS to fulfill its mission. The key components to consider are as follows:

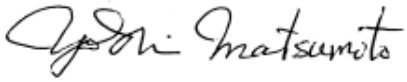
1. Activity of IMS during the period of present DG (From April 2016 till present)
   - 1-1 Science activity of IMS as a whole
   - 1-2 Organization of IMS, such as Divisions, Research Centers and other activities
   - 1-3 Revitalization of IMS measured
   - 1-4 Activity as the Inter-University Research Institute
     - 1-4.1 Activity of the joint research projects and the shared facilities
     - 1-4.2 Organization of the joint research systems
     - 1-4.3 Revitalization measured
2. Advice on the future perspective for IMS

The IMSAC is also asked to advise on the suitability of IMS as the Inter-University Research Institute, referring to the guideline given by our Government. (Expecting Guide Line shown in the Additional Report from Director General)

The members of IMS Advisory Council are:

Yoshiyasu Matsumoto, chairman	Toyota Physical and Chemical Research Institute
Peter J. Rossky, vice-chairman	Wiess School of Natural Sciences, Rice University
Akira Hiruma	Hamamatsu Photonics K.K.
Tetsuya Ishikawa	RIKEN SPring-8 Center
Noboru Kikuchi	Toyota Central R&D Labs, Inc.
Benjamin List	Max-Planck-Institut für Kohlenforschung
Hatsumi Mori	The Institute for Solid State Physics, The University of Tokyo
Ron Naaman	The Weizmann Institute of Science
Masashi Takigawa	The Institute for Solid State Physics, The University of Tokyo

This advisory report reviews the current situations of IMS and describes various suggestions from the IMS Advisory Council. We hope that this report helps IMS for further growth as a worldwide center of molecular science research.



Yoshiyasu Matsumoto
Chairman of IMSAC

1. Science Activity of IMS

The mission of Institute for Molecular Science (IMS) is to promote the progress of molecular science that currently covers a wide range of research topics, through mutual exchange of human resources between domestic universities and through international collaboration with the world's scientific society. For this purpose, IMS has been actively fostering many joint programs, with the aim of establishing a research core in advanced molecular science. IMS has been providing maximum opportunities for collaborative research and full utilization of its state-of-the-art facilities by all Japanese researchers in the field and building a robust research network among the international scientific community.

IMS consists of four departments as a concrete foundation of molecular science, two research centers representing research foci at present, four research facilities to support research teams, and two divisions exhibiting advances of the field scientifically and socially. Moreover, Exploratory Research Center on Life and Living Systems (ExCELLS) has been established to integrate knowledge from the three institutes of NIBB, NIPS, and IMS, in the quest for the secret keys to life and living. The challenge of IMS continues.

1-1. Department of Theoretical and Computational Molecular Science

The Theoretical and Computational Molecular Science group derives from its foundational role in the development of IMS. It began with the appointment of quantum chemist Keiji Morokuma as the Founding Director of the Department in 1977, the nomination in 1982 of theorist Iwao Ohmine as a young associate professor (and later the seventh Director General), and the promotion of IMS Prof. Hiroki Nakamura, a theoretical chemical dynamicist, as the sixth Director -General of IMS.

The present Department has evolved a great deal from these days, with a broad range of current topics represented by the present faculty. The issues pursued by the theory group represent an excellent balance across the current frontier topics in the area. Specifically, there is a strong representation of condensed phase molecular science, including nanoscale materials and biomolecular systems, of dynamics including quantum systems, and of electronic structure theory with advanced applications of new methods that are opening up access to complex molecular systems at an accurate *ab initio* correlated electron level. Noticeably missing are individuals who are making only incremental contributions to problem areas that are primarily addressed by earlier work. This absence shows the strength of the group on an international scale.

Of primary importance, the theoretical and computational research now going on at the IMS is uniformly excellent and represents in every project, research that is of world-class. The problems being attacked are at the frontiers of science, and the approaches are cutting edge. There is no gap between the research topics represented at IMS and those of primary focus in Europe or the USA. The self-awareness of their competitive position as scientists in the broad perspective is

outstanding. Most importantly, individuals are global scientists, who are knowledgeable about the worldwide network of theoretical and computational molecular science. This represents an enormous change from the early years of IMS and a notable evolution continuing even during the past five years. We attribute the attainment of such a high point of success to outstanding leadership.

It is essential for the individuals in the Theory group, in particular, not to miss the current wave of participation in the AI/Data Science world. Molecular theorists, who also have refined mathematical and computational skills, are uniquely capable of implementing such methods in very relevant and impactful contexts, an ability missing from individuals trained as AI experts but without "molecular intuition."

Regarding organization, the success of the deployment of Prof. Okumura as a joint appointment in the ExCELLS research thrust points to a more general opportunity. The embedding of theoretical scientists within topical experimental research groups typically stimulates opportunities for collaborative science that remain unrealized when these skills are separated. The embedding increases the impact of both experimental and theoretical efforts. Such integration of theorists should be considered more generally, in consultation with project leaders and principal investigators. We believe this would be well received by all involved and would be particularly valuable for the interpretation of data in cutting-edge areas such as single-molecule spectroscopy and advanced imaging.

1-2. Department of Photo-Molecular Science

This department aims for (1) developing light sources including synchrotron radiation, (2) facilitating new spectroscopic methods, and (3) studying the properties, functionalities, and reactivity of materials. The works of each PI group are excellent, and some are at the forefront of science.

(1) Development of light sources: UVSOR is the largest facility in IMS, dedicated to UV and soft-X ray range. In the past, the facility has undergone continued refurbishment and improvement to be competitive with the other synchrotron light sources providing light in a similar range. The enormous effort paid for this optimization and development of lower emittance deserves admiration. The group in UVSOR has been working actively in developing new light source technologies, including generation of structured light and a laser Compton scattering gamma-ray source.

(2) New spectroscopic methods: The department has succeeded in developing new spectroscopic methods. It is fascinating to see the cutting-edge research to develop a quantum simulator using a coherent control technique targeting an ensemble of ultracold Rb atoms in Rydberg states. This project depends on impressive former achievements, including coherent control in the gas phase and solid para hydrogen. Also, various kinds of x-ray spectroscopic methods have emerged with UVSOR that enable identification of local chemical states of specimen. In particular, the application of x-ray absorption spectroscopy to liquid and liquid-liquid interface is

impressive.

(3) Characterization of materials: IMS has been one of the core institutes in the field of organic semiconductors since the former Director-General Prof. Inokuchi conducted the project of organic semiconductors, intensively. This tradition continues. As an in-house activity, measurements with high precision have been done on the electronic structure of functional organic molecules at surfaces and interfaces by using angle-resolved photoemission spectroscopy (ARPES).

Therefore, the department has achieved excellent progress addressing all the three aims. However, the department suffers from a shortage of research groups. It is necessary to hire new PIs to reinforce the department; alternatively, IMS needs a grand design for the near future to restructure the department accordingly.

1-3. Department of Materials Molecular Science

Some of the research subjects missing in the department can be adapted by collaboration with other laboratories, but it is essential to have 2–3 people that are in the material synthesis community and can help in matching research groups from outside the IMS with the groups internal to the department.

Given the central role material science is playing in modern science, the department must be strengthened significantly, and its size should be doubled. It is indeed essential to keep the high standard of hiring, but it is also important to widen the research topics. If possible, it will be useful to hire people that spend time in leading labs outside Japan, or even foreigners, so that the ties between the department and the international community will be tightened. Also, one should consider including in the department a theoretician working on electronic and magnetic properties of materials. Such a theoretician could collaborate with the experimental groups.

A possible approach is to combine the department with other departments and to establish a more substantial department for “Chemical Physics”.

1-4. Department of Life and Coordination-Complex Molecular Science

The overall impression of the Department of Life and Coordination-Complex Molecular Science is excellent. It is suggested to consider finding a more appropriate name for this department, for example, “Complex Molecular Science”, if IMS holds the current many small departments (see the other suggestion regarding the reconstruction of departments in 3). The PIs in this section tackle various grand challenges, ranging from the study of the physical properties of extended π-electron systems, over super high-performance catalysis, ultimately to the self-assembly of living systems. Considering the breadth of the scientific investigations covering physical chemistry, chemical synthesis, inorganic and organic chemistry, materials chemistry as well as biochemistry and chemical biology, strategically, hiring at least one additional PI, in the broader area of synthetic chemical biology/biochemistry, is recommended. He/she could help make the bridge between the

more biology-oriented activities (for example by Prof. Kato) and those that are more chemical/material/chemical physics-oriented. The already consummated recruitment (Assoc. Prof. Kusamoto, who will work on open-shell molecules) and those that are planned (probably in the area of chemical synthesis of π-systems) are highly promising.

1-5. Research Center of Integrative Molecular Systems (CIMoS)

The Center aims at strengthening the research performances of IMS, as part of a globally competitive strategy. The research center aims not only to reveal the underlying rationale for the behavior of individual molecules and molecular assemblies in terms of molecular science but also to create and to study new molecular systems and their structural and electronic properties. The research themes the people in the center pursue are highly sophisticated and internationally competitive, and the level of engagement of each member is quite intense in terms of research activity. The atmosphere in the center and the physical setting support the exchange of ideas among both the senior faculty members and the students. It is expected that the significance of the center will further increase, with the introduction of frank and candid exchange of views among the research groups. Some creative collaborations between laboratories have already begun, with high expectations for paving the way to state-of-the-art research fields. The center is serving as an excellent example of how to organize interdisciplinary research.

1-6. Center for Mesoscopic Sciences (CMS)

The focus of this center is stated to be "to elucidate the processes that trigger the functions and reactions of molecular systems in the mesoscopic regime." Up to now, the center has developed a method for generating and controlling the chiral optical field. This method would be beneficial for analyzing handedness in molecules and nanocomposites. Usually, circular dichroism (CD) is challenging to detect. The development of CD microscopy makes it possible to apply this method to materials in the mesoscopic range. Despite the impressive growth, it is difficult to see how the center is organized to produce cutting-edge research work. The center needs to clarify its vision and select the right PIs to fit. Communication among the people in the center and collaborative practices are highly encouraged to meet the goal of the center.

1-7. Division of Advanced Molecular Science

Thanks to the strong leadership of the current Director-General, a new division, Division of Advanced Molecular Science, has been established, which allows a distinguished scholar to have an opportunity to maintain his/her research activity in IMS even after mandatory retirement in university. It is noteworthy that Distinguished Prof. Fujita, invited to this Division, used to work in IMS as an associate professor. He has achieved outstanding work on self-assembled molecular

systems based on coordination chemistry. Furthermore, he has recently developed a versatile method for structural analysis of molecules, crystalline sponge method, which does not require crystallization of samples. This Division helps to significantly increase the scientific visibility of IMS.

1-8. Division of Research Innovation and Collaboration

IMS has been one of the leading institutes in Japan for both experimental and theoretical research. Moreover, IMS has initiated a program in which they focus not only on academic research but also on innovation working with industry. TILA (Tiny Integrated Laser) consortium is such a program, yielding a micro solid-state laser advancement and creating an industrial application that will maximize the benefit of research results and meet industry needs. The advance of laser technology has provided many applications, and we have been benefiting from them, such as distance measurement for construction, eye surgery, and satellite-based atmospheric research. The integration of a tiny microchip laser with high power and stability will give us much broader application possibilities. With it, even a tabletop accelerator could be possible, which could bring new scientific research.

The time is ripe to have stronger and more coordinated work between academic research organizations and industry to find more advanced usage for these high power lasers.

It is essential to reorganize the current Industry-Government Agency-Research/University relationship to realize such collaboration. We need a research organization to advance the science, government agency to fund the research and industry to commercialize the technology. However, top research organizations have very little time to convert their science to the technology that many companies can use. Meanwhile, some local universities in Japan have limited talent to advance science but have a significant responsibility to contribute to local industry advancement. Therefore, it may be best to expand the current three-way Industry-Research/University-Government collaboration (I-R-G) into a four-way relationship: Industry-Research/University (Science)-Local University (Technology)-Government agency (I-S-T-G). The essence is already evident in the TILA consortium. Including local technological universities to focus on actual applications of tiny microchip laser for small-to-medium companies may lead to new applications in more extensive areas.

2. Activity of the Shared Facilities, ExCELLS, and the Joint Research Projects

IMS houses open-use research facilities to promote the discovery of molecular behaviors and properties. Four facilities have been settled: (1) UVSOR Synchrotron Facility, (2) Instrumental Center, (3) Equipment Development Center, (4) Research Center for Computational Science. Moreover, (5) Exploratory Research Center on Life and Living Systems (ExCELLS) has been recently established. With these facilities and the organization in addition to (6) Joint usage and joint research projects, IMS promotes collaboration with universities and research institutes around the world.

2-1. UVSOR Synchrotron Facility

Prof. Umbach's assessment report provides a comprehensive analysis of possible future courses for the UVSOR facility. It is entirely up to the IMS management decision which option the Director-General would take, but we would add some information that may help to make the decision.

The present UVSOR is not very far from the ideal 'diffraction-limited light source' because of the continuous improvements made so far. The problem is not the light source performance, but the aging of components which could deteriorate the stability and reliability of the facility. Almost no new development is necessary to refurbish the light source itself. Therefore, the upgrade cost would not be very high.

The unique position of UVSOR in the Japanese synchrotron radiation (SR) research community is that it is the facility for chemistry. Although there are six operating SR facilities in the low energy range like UVSOR in Japan, UVSOR is the only facility serving mostly academic users, including many chemists. Some people are considering a league among SR facilities for academic users, Photon Factory, UVSOR, and HiSOR as an entity to negotiate with MEXT. It requires a thorough analysis of what this cooperative 'league' will bring.

From a different point of view, UVSOR could be a low energy member of the Japanese advanced SR facilities with nearly diffraction-limited performance. SPring-8 will cover the high-energy part, and the Tohoku new 3 GeV facility will include the mid-energy part. This direction may open up a possibility to operate UVSOR under the 'Act on the Public Utilization of the Specific Advanced Large Research Facilities' as are SPring-8 or J-PARC.

The 'weight' of chemistry is increasing in the SR research community. The reason for this is that not only academic users but also industrial users are growing at a high pace. Internationally, many pharmaceutical industries are participating in SR researches. However, not only the pharmaceutical companies but also many polymer companies have jumped into the SR research in Japan. In considering the future direction of UVSOR, it may be essential to decide whether the facility would include more industrial users or not. This decision is strongly related to the future

standing point of UVSOR in an academic league, or a diffraction-limited facility league. Technically, UVSOR can serve the structural biology community by installing some new components.

That said, UVSOR is a conventional light source that can serve general users who may not be familiar with the synchrotron radiation. The number of users from IMS is decreasing, while the outside users are increasing. The management principle of the facility should move to a more 'user-oriented' focus. A short-term solution could be to maintain the present UVSOR while applying the patches. However, IMS should have a concrete mid-term or long-term vision on the light source facility. We recommend setting up an internal task-force to make a plan for UVSOR in collaboration with the user community. A broader discussion in the landscape of the Japanese SR community may also be necessary.

2-2. Instrumental Center

Missions of the Instrument Center are: (1) to promote the state-of-the-art instrument and to maintain necessary conventional equipment for in-house and external researchers, (2) to manage three projects as representatives for promoting joint-research/joint-use. The plans are "Nanotechnology Platform Program (Platform of Molecule and Material Synthesis)" by The Ministry of Education, Culture, Sports, Science and Technology (MEXT), "Inter-University Network for Efficient Utilization of Research Equipment (Equipment NW)" by MEXT, and programs in National Institutes of Natural Sciences (NINS)–Inter-University Cooperative Association (NICA).

The recent improvement of the instrument center is an increase in the number of members for strengthening the system of joint-research/joint-use. Two team leaders (TLs), Dr. Toshikazu Nakamura (analytical TL), and Dr. Toshiyasu Suzuki (synthetic TL) joined to support and promote research with in-house and external researchers.

As for instruments, a new E-beam lithography system was settled in 2018 and is taken care of in Equipment Development Center, and a local micro-probe system will be set in 2020. On the other hand, there are still old apparatuses, which were introduced more than 20 years ago: e.g., MPMS-SQUID (Magnetic Property Measurement System-Superconducting quantum interference device) and PPMS (Physical Property Measurement System). In-house and external researchers have commonly utilized these apparatuses. It is recommended to plan for updating the old conventional and useful machines and appliances. Recent MPMS-SQUID and PPMS with recycling He systems might be helpful to save Liq. He.

2-3. Equipment Development Center

In the Equipment Development Center (EDC), various pieces of experimental equipment necessary for molecular science research have been manufactured and developed. This EDC is composed of the mechatronics section, electronics section, photolithography section, and digital engineering section, where technical associates and technical fellows with advanced technology and

skills have been working. Since the establishment of IMS, technical associates have worked closely with researchers inside and outside IMS to develop various experimental devices and instruments that enable their original research. Workshops on machining, electronic circuit work, and micro-machining are open to researchers and students to disseminate technology.

The mission of EDC is to work strategically as a central technology hub to develop molecular science by responding to the requests of researchers.

The ability of the technical staff is essential to utilize and maintain the new experimental equipment. It is practical to give the technical associates incentive like special salary to employ and keep superior technical associates with specialized techniques in this EDC.

2-4. Research Center for Computational Science

As a national shared computer center, the Research Center for Computational Science (RCCS) provides an advanced computational environment and libraries to about 150 groups of domestic molecular/biomolecular scientists with a very large-scale calculational resource that would be difficult to create on one university's home ground.

The RCCS provides state-of-the-art computational resources to academic researchers in molecular science and related fields, e.g., quantum chemistry, biomolecular simulations, bioinformatics, and solid-state physics. The computer systems consist of multiple NEC CPU and GPU clusters with a current estimated total peak performance of 4 Pflops. Also, there is a developmental Fujitsu Server with an architecture that mimics that of the "K computer."

The Computer Center of IMS, which was the forerunner of the RCCS, was established in 1977, primarily to provide an opportunity for large scale computation in molecular science, which could not be carried out at regional university computer centers. Further, the Center supported experimental data collection and analysis, developed and maintained the program library and database in molecular science, and provided the computational service to neighboring National Institute for Basic Biology and National Institute for Physiological Sciences.

In 2000, the Center was reorganized into the RCCS of the Okazaki National Research Institutes to extend its activity to the frontier between molecular and biosciences. Since then, the Center has also been engaged as a partner in science by developing new theories and simulation methods. After 2004, when Okazaki National Research Institute, itself, was reorganized into the National Institute of Natural Sciences, the Center has been active as a member of Okazaki Research Facilities.

The Center is managed and operated by a faculty oversight committee, traditionally led by one or more members of the Department of Theoretical and Computational Molecular Science, continuing the tradition, since the founding of the computational resource, that the head of that department has a unique role within the RCCS leadership. There is, also, a substantial professional staff that provides a consistently excellent and reliable service to a large number of users (typically ~700 individual users on an annual basis).

The role of this Center in the success of the IMS has been critical and is increasing as

computational materials science, computational biology and biophysics, and the long tradition of computational chemistry play increasingly more significant roles in science and engineering. It is evident in the fact that the RCCS has been a *critical asset* in obtaining large projects for IMS that involve computational scientists and that bring significant funding for computational resources. In particular, the Center made a substantial contribution to the project, "Grid Application Research in Nanoscience," by IMS as a grid computer center, which was a part of the activity of the national project, "National Research Grid Initiative (NAREGI)," by MEXT, Japan, from 2003 to 2005. Now, the Center is working as a significant component of the project, "Development of New Computational Methods for Large-Scale Systems and Establishment of Bases for Advanced Simulation of Molecular and Material Systems," by IMS forming a part of the project, "Formation of Interdisciplinary and International Bases Across Fields of Study," by NINS. The Center is playing an important role, too, in the national project, "Grand Challenge to Next Generation Nanoscience," by IMS in "Development & Application of Advanced High-Performance Supercomputer Project" by MEXT, Japan.

2-5. Exploratory Research Center on Life and Living Systems (ExCELLS)

A key goal laid out by Director-General in her report to the IMSAC is for the IMS to be the nexus for collaboration between universities and across NINS. The Inter-university Research Institute Corporation appears to have been set up to promote this function, here through the National Institutes of Natural Sciences (NINS). However, the NINS "Collaborative Research Map" and the descriptions of such efforts are uniformly vague, and evidence of collaboration from previous reports is essentially all anecdotal.

This situation may change. The Exploratory Research Center on Life and Living Systems (ExCELLS) was launched in April of 2018 directly under the National Institutes of Natural Sciences. As it is relatively early, a thorough evaluation of this center cannot yet be conducted. However, the concept of the center and the personnel it has assembled are of outstanding potential.

The hugely ambitious ultimate goal of the Exploratory Research Center on Life and Living Systems is to answer the question, "What is life?" Within ExCELLS, new approaches to observing biological entities, for example, under extreme conditions, to the deciphering of hidden information through big data analysis, and ultimately to creating living systems, will be developed. Furthermore, ExCELLS is specifically designed to promote interdisciplinary research collaborations between different investigators. The center covers a topic of utmost current interest and has a genuinely outstanding potential for successfully contributing to some of the grand challenges of science.

Dr. Koichi Kato directs the center, ExCELLS, whose individual highly interdisciplinary scientific program has been described in the context of the Department of Life and Coordination-Complex Molecular Science.

A question that arose was how all the extraordinarily diverse and interdisciplinary activities

could be focused on a common goal. The "Golgi Atlas" project, to which many of the groups can contribute at least in principle, appears to be a good starting point for such efforts. Prof. Kato personally emphasized that he considers his role as the director of this program to unite the different research activities and groups. Considering how he leads his research department, there is little doubt that he will be at least as successful with the current center ExCELLS.

2-6. Joint Usage and Joint Research Projects

Joint-research/joint-usage is a vital mission for IMS as one of the institutes affiliated with the Inter-University Research Institute Corporation in Japan.

There are several joint-usage and joint-research projects in IMS as follows:

(1) Large network-type projects funded directly by the government:

(1-1) 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." This post-K computer program will terminate on Mar. 31, 2020. The following program needs to be planned to promote computer science.

(1-2) MEXT Nanotechnology Platform Program, Platform of Molecule and Material Synthesis. This program started in July 2012 to promote public usage of various nanotechnology facilities and lasts until Mar. 2022. This program is recommended to be continued to encourage joint-research/joint-usage.

(1-3) Inter-University Network for Common Utilization of Research Equipment. This program was launched to construct a nationwide network in 2007. As of June 2019, the number of registered users amounts to 13,000 from 385 universities/institutions/companies covering over 3,500 laboratories in Japan. Since this program is practical and useful for researchers in Japan, it should be planned to be continued in the future.

(2) Small-size projects supported by IMS:

The joint studies programs (special projects, research symposia, joint studies program), the international Okazaki conference, and international and inter-institutional collaboration symposia have been carried out as the joint-research/joint-use institute. To promote the globalization of the institute, various kinds of flexible international programs, such as short-term (1-2 months/year for several years) visiting foreign professor program and short visiting researcher program might be useful. It is also recommended to actively invite female international researchers to maintain the diversity of human resources in IMS.

One crucial thing that appears missing at IMS is a *quantitative* record of collaboration; data on collaborative grants, collaborative papers, co-supervised researchers, and so on, can provide evidence for such interactions or their absence that can be tracked and used by Department heads/Center Directors.

3. Revitalization Strategy Measured

The current Director General (DG) presented the initiatives she has taken from 2016 to revitalize the institution. Her foci were to bring in some senior scientists to attract the community and general society to increase the scientific visibility of the institute.

Along this line, the DG has introduced new Divisions. Among them, the establishment of Division of Advanced Molecular Science, in which Distinguished Prof. M. Fujita has been invited as a PI, will lead to the significant success for reinforcing the scientific visibility of IMS. It would be advisable to invite more distinguished professors to raise the IMS profile even higher. Also, hiring scholars from abroad will be much encouraged. There might be some technical difficulties concerning salary, housing, or other things, but OIST (Okinawa Institute of Science and Technology Graduate University) will be a good practice model to enhance the globalization of IMS.

Setting Division of Research Innovation and Collaboration attracted the local community of innovation. Major invention of tiny solid laser by Project Prof. Takunori Taira has advanced to the phase of change, which excites private companies, leading to collaboration with society.

The organization of the Institute has too many and too small departments. Restructuring the current departments is highly encouraged; for example, one could divide all the existing departments into two departments: one is physical molecular science, and the other is soft matters chemistry (or molecular life science).

It is also essential to reinforce the section of university-research-administrators (URA) to reduce the burden of particularly full professors in IMS, which allows them to concentrate on their research projects as described in 4-1.

As one of the Inter-University Research Institutes, IMS needs to promote cooperative researches with scholars in universities. For this purpose, the DG has established the Division of Intensive Research, where IMS invites adjunct professors to develop new ways to use facilities of IMS. Hiring Dr. Matsui as a Senior Researcher in the UVSOR facility helps support the activity of UVSOR. Otherwise, the shortage of researchers and technical staff in the facility makes the operation and update planning of the facilities more difficult. Moreover, as described in 2-1, IMS should have a concrete mid-term or long-term vision on the light source facility.

The current DG has reassigned the jobs of a couple of associate professors, which has not been done by any former Director Generals: Dr. Shigemasa was reassigned to the Head of Technical Division, Dr. Nakamura to the team leader of Analysis team and Dr. Suzuki to that of Molecular Synthesis team in the Instrument Center. These reassignments are expected to further enhance the activities of cooperative researches with scientists from outside universities and research institutes.

Another particular example of change is new flexibility in the hiring process. Prof. Ishizaki and Assoc. Prof. Kobayashi were hired under non-traditional terms, where they could be promoted and stay at IMS, rather than being required to move to another organization. Also, recently, positions have been opened to international candidates. These are quite positive changes in terms of enabling the development of the most influential possible group of scientists at IMS accessing the

open global marketplace.

We note that the Department of Theoretical and Computational Molecular Science and the Department of Life and Coordination-Complex Molecular Science have hired a few female faculty members of the IMS, an important step. The relatively new and cross-cutting ExCELLS group appears to be the only one that has a significant female representation, by international standards. It would be invaluable to the Theory group's apparent broad role in leading the standard for theoretical chemistry in Japan if the group were able to identify and hire additional female faculty in this field and, particularly, entry-level female faculty. These individuals would serve as appealing role models that could place the Department in a position to take a leadership role in actively attracting female graduate students in the broader physical sciences, in a virtuous cycle.

4. IMS as the Inter-University Research Institute

Institute for Molecular Science (IMS) is one of the 17 institutes specified as Inter-University Research Institute Corporation. The fundamental mission of these institutes is to contribute to the development of academic research at universities or to support them by maintaining large facilities necessary for shared use among scientific communities.

IMS is required to have a suitable shape as an Inter-University Research Institute in terms of the following seven components.

4-1. Administration

The administration and operation of IMS, as well as the process of recruitment of researchers and faculties, are transparent to the research community to meet the fundamental mission of Inter-University Research Institute Corporation. Also, IMS maintains communication channels accessible to the researchers of molecular science so that IMS can adequately consider their opinion for better operation of the institute. It is essential to enhance cooperative researches in IMS with outside scientists in various established sub-fields of molecular science.

At the same time, it should be equally important to explore new directions and encourage collaborative challenges between researchers with different expertise and knowledge to create new sub-fields of molecular science. IMS should have mid- to long-term strategic plans for future initiatives along with new directions and make priorities in the use of its resources. It will be helpful to have an informal board of people who can give thoughts to the director and the senior managers of the institute to decide which areas to focus on various possibilities. They may not represent the majority of the molecular science researchers but should have specific views on what would be the promising fields to pursue.

The effectiveness of administration is an important issue. Senior faculties of any major institute in Japan are now required to spend a significant amount of time and effort for administration. As a result, they are challenged to find sufficient time for their research. Their commitments are necessary when an important decision has to be made. However, they should be freer from other administrative duties such as institutional research, some aspects of public relations, and proposing funding agencies. For this to happen, one of the critical elements would be the addition of one or more talented university-research-administrators (URA) who can handle such tasks as collecting information and analyzing statistics of the relevant research fields and communicating with community or funding agencies. Since the URA system in Japan started relatively recently, only several years ago, those in the early stage of the career need to have a senior partner to consult.

The employment system of researchers has changed dramatically in Japan for the past twenty years. At IMS, internal promotion used to be strictly forbidden. However, a variety of career paths with various degrees of independence for young scientists is now available with successful examples. Such flexibility in hiring and promotion would be generally encouraged.

4-2. Core Institute to lead the community for Molecular Sciences

IMS was established in 1975 as a research institute under the direct control of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), aiming to become the center of excellence in the scientific field of molecular science. IMS now belongs to Inter-University Research Institute Corporation, National Institutes for Natural Sciences. Many Japanese researchers in the field of physical chemistry had been a member of IMS, so that IMS has produced many outstanding physical chemists.

IMS has worked as the core research institute of molecular science for the past 44 years, conducting cutting-edge researches, joint-research/joint-use, holding symposiums on recent research topics, and various issues, including research environment, and organizing projects such as research equipment networks for leading molecular science research.

The researchers in the field of molecular science demand both standard and cutting-edge equipment for their research. Owing to the reduction of the budget in the national university and less supply of liquid He, the standard equipment is necessary to maintain the research activities and to support researchers. Also, cutting-edge equipment and facility, which a university cannot manage, are essential to promote novel molecular science.

The large facilities in IMS are UVSOR light source facility and computational center. The low-energy SR (<1 GeV) is an essential facility for solid-state scientists to determine the band dispersion, which cannot be covered by laser and other facilities. It is of importance to discuss the benefit of UVSOR for cutting-edge research in addition to the common usage in the scientific field of chemistry by comparing to other world-wide SR facilities.

Since IMS currently has Yamate campus besides Myodaiji, it has a more substantial area but a smaller population than in the old time. IMS needs to make a strategy to involve external scientists in the activities in IMS; for example, the quantum chemistry and computational school in IMS should keep attracting students and academic and industry researchers.

Looking ahead to the next 50 years, it is essential to continue the discussion about the direction of IMS as the core research institute in the field of molecular science.

4-3. Institute as an International Core

Based on high reputation of IMS in international research communities through their world-class high-level facility as well as research activity known through journal publication, IMS annually organizes Okazaki Conference in which prominent leading core researchers in Molecular Science are invited from oversea countries, while international and inter-institutional collaboration symposia are also organized both in Japan and overseas. Furthermore, between 2018 and 2019, 22 participants are counted in IMS international internship programs, two students from abroad, in addition to nine foreign internship students participated to SOKENDAI Asian Winter School, and over 100 researchers are counted in the international joint research program and global use of

facilities program. These facts show IMS's high reputation as an internationally well-recognized core institution in Molecular Science.

To build up further the high reputation of IMS as an international core, for example, it may be suggested that at least one or two regular faculty positions in IMS are intentionally assigned to non-Japanese scholars who can facilitate diversity of IMS activity both in Japan and in overseas. It naturally implies that their research activity would be published in every IMS annual report so that IMS diversity can be recognized internationally. Since IMS has already established close collaboration with many European and Asian institutions, including universities, IMS may exchange sabbatical leave programs so that their faculty can work in other oversea institutions in a rather long period to promote deeper collaboration in research. Foreign faculty naturally invites international students and post-doctoral students from abroad, and he/she also assists the mixing of talent internationally.

4-4. Research Resources

The *required mission* advocates the ideal situation for research resources. This is quite common for this kind of statement. When assessing what is happening from the statement of *our mission*, it should be acknowledged that the IMS runs shared facilities that are too large to be managed by a single university, and at least intends to perform maintenance and the appropriate renovation of the facilities to promote active use by the scientific community.

The Report from the DG of IMS addressed the various scales of large shared facilities. Among them, it may be necessary to discuss in more detail the two largest facilities, UVSOR and Computational Resources. High-power computational resources are distributed across many places in Japan. The hardware development is mostly performed in the industrial sector. Therefore, the academy comprises mostly of users. It seems not so difficult to keep the computational resources if the appropriate budget is secured. However, a synchrotron radiation facility like UVSOR developed in the academic sector demands each managing institute to provide operating and developing staff. If the IMS plans to start a large-scale upgrade of UVSOR, the current number of accelerator personnel is far less than will be needed.

Each Inter-University Research Institute Corporation has a mission to manage the shared large facilities used mostly for academic research at universities. Significantly increased demand from industrial communities would always present a challenge for these facilities. The IMS should scrutinize the present situation with UVSOR to determine whether the current management scheme is appropriate. In particular, global competition is growing in synchrotron radiation research, accompanied by an accelerating technical revolution of light sources. Much more frequent upgrades are required to keep up with global trends.

More open shared facilities, notably including the industrial sectors, are supposed to be the responsibility of National Research and Development Agencies like RIKEN (SPring-8 & SACLA, K-Computer), JAEA (J-PARC), and QST (New SR facility in Sendai). These agencies, like

the IMS, are overseeing the operation of shared facilities (customer-oriented service) and basic research (pursuit of self-interest) simultaneously, without making a clear distinction between different managing principles.

A thorough examination should be necessary to make the different managing principles compatible within a single institute when the IMS decides to conduct a globally competitive upgrade of UVSOR.

4-5. Commitment to innovate new area of science

IMS commits itself to cultivate new fields of science, particularly in molecular science, which is achievable with new ideas of researchers in IMS and enough funding to realize these ideas. Also, recruiting researchers with potent capabilities is necessary. IMS has provided an excellent opportunity for young and talented researchers to make their independent group. The validity of this system can easily be recognized if one considers that many former IMS associate professors have obtained full professorships in decent universities and work as leaders in the field of molecular science. The spirit of this IMS continues in the term of the current Director-General: IMS has recently hired talented young researchers as associate professors such as Drs. Kobayashi, Sugimoto, Minamitani, and others.

In the coming several years, several professors will be retired. Thus, IMS meets the time of necessity to reform the structure and prepare for opening new fields. IMS and its community should survey the current activities in molecular science and related areas to plan future directions for IMS to cultivate. IMS should not hesitate to hire non-Japanese scholars if it is needed for fulfilling this purpose.

4-6. Cultivating personnel

IMS has been very successful for growing, particularly young researchers, for example associate professors. As stated earlier, many former associate professors of IMS have been promoted to be full professors in decent universities and institutional labs. A symbolic example is Distinguished Prof. Fujita, who used to work as an associate professor in IMS, is now a Professor at the University of Tokyo and the PI in Division of Advanced Molecular Science in IMS.

In contrast, IMS has been struggling to have graduate students. This is the structural problem in this country, and has not been changed and will be challenging to change in the short term. The decrease in the number of students in Japan makes the situation even worse. As pointed out during our discussion, IMS should recruit international students who are highly motivated to do Ph.D. works in molecular science. For this purpose, IMS needs to have the right tactics to attract international students, including the advertisement of the institute and preparation of special scholarships enough for international students to live in Okazaki.

4-7. Relation to Society

For an Institution like IMS, it is a top priority to focus on cutting-edge scientific researches. However, to get general public support for the institution, it is essential to share their research topic with the general public in plain language that is easy to understand. For that, it is good that IMS is hosting seminars for public forum titled “Molecular Science Forum” four times a year. They are also accepting group tours to show the model of their vast research machine. Such public relations should be encouraged.

Also, the program like TILA consortium, connecting the top research to actual industry for open innovation, is essential. To advance the concept further, IMS may be willing to have some industry incubator program so that researchers themselves venture into making startup companies. The activity like the TILA consortium may lead to further innovative activity as potential startups. Large companies would be willing to invest in such a startup by sending engineers as well as providing seed money needed. Researchers at IMS could be CTO or top scientific advisers while engineers from a company being CEO.

If it is too much deviation for IMS to take the road toward making their own incubator, it would be desirable for researchers to take a post of scientific adviser for such startup companies. Many companies, either large established companies with a new project or startup companies, can appreciate such help.

Mentioning about the effects of basic science on our society, it is not apparent whether or not basic science will provide an immediate impact on society. But a study like quantum simulator work by Prof. Ohmori’s group could potentially offer us a massive benefit to the future of our society by a deeper understanding of the quantum world, which may lead to the advancement of quantum computers. Although the work, such as Prof. Ohmori’s, is the basic research that may bring us breakthrough knowledge, society should not look for a quick return.

5. Summary and Suggestions

IMS has been keeping research activities of world-class, and many of the problems being attacked are the frontiers of science. The current Director-General has made new attempts to make IMS more visible scientifically, including the establishment of Division of Advanced Molecular Science, where a distinguished scholar of another organization is invited to open a new lab also in IMS. This widens the research area of the Institute and allows the renowned scholar to perform a cutting-edge project even after retirement from the current organization. This win-win situation surely helps to raise the scientific visibility of IMS.

Despite the success in research accomplished in IMS, the Institute has a few problems to be overcome soon. First, the Institute needs to have a concrete mid- or long-term vision on the UVSOR facility. This kind of a large-scale facility is critical for an Inter-University Research Institute. Second, the Institute is facing the time to reform the structure of the Institute and to prepare for opening new fields as several full professors will be retired in several years. It is advisable to start planning for future directions of the Institute. Third, accepting foreign researchers is also a vital issue for increasing the presence of the Institute. IMS should have more foreign researchers and Ph.D. students. Having Japanese graduate students is going to be more difficult because of a decrease in the number of students in Japan. Hiring non-Japanese professors may encourage superb international students to come to IMS. Henceforth, also for this purpose, IMS should manage to improve the research environment for a full professor to attract talented scholars all over the world. It is advisable to change the management system for separating administrative works from the scientific activities of full professors.