７．点検評価と課題

2022 年度より James M. Lisy 教授（イリノイ大学）と北川　進教授（京都大学）に研究顧問に就任頂いた。2022 年 5 月開催の IMS Presentations 2022 に Web 参加頂き，所全体の研究評価，研究体制についての提言をいただいた。

2023 年 3 月には，新型コロナウイルスによる感染者の大幅な減少を受けて，ハイデルベルグ大学の Matthias Weidem 教授に来所頂き，光分子科学研究領域を中心ヒアリングが実施され，各グループの研究内容と極端紫外光研究施設（UVSOR）の評価をいただいた。同じく 2023 年 3 月に，マンチェスター大学 David A. Leigh 教授が来所し，生命・錯体分子科学研究領域を中心にヒアリングが実施され，各グループの研究内容の評価をいただいた。

2023 年 2 月に Web で開催された運営顧問会議では 2022 年度に実施した特任教員などの新たな雇用制度等，就任 1 年目の運営上の課題について議論頂いた。

（渡辺芳人）

7-1　運営顧問による点検評価

運営顧問から第 4 期中期計画期間での運営方針のためのアドバイスをいただくことを目的として，3 名の運営顧問を招いて運営顧問会議を開催した。

分子科学研究所の第 3 期中期計画期間の活動については，2019 年 12 月から 2021 年 7 月にかけて機関の点検・評価が行われた。その結果については，分子研リポート 2019 において，7-1 国際諮問委員会による点検評価，また分子研リポート 2020 において，7-1 大学共同利用機関の教育研究等の検証，7-2 国際諮問委員会の答申リポートとして公開されている。また，2021 年度に実施された運営顧問会議の議論内容が，川合前所長から申し送られている。これらを踏まえ，分子科学研究所の抱える課題とそれらへの対応状況を，渡辺所長から運営顧問に説明した。会議当日には，第 4 期中期計画期間での研究所機能強化に向けた機関運営方針の提案・検討事項について運営顧問から意見をいただき，渡辺所長の考える改革案に対する支持とアドバイスが表明された。

1. 日　時：　2023 年 2 月 27 日（月）10:00 ～ 11:00
2. 方　式：　オンライン開催（zoom 会議）
3. 出席者：

運営顧問

菊池 昇　（株式会社コンポン研究所 代表取締役所長）
長我部 信行　（株式会社日立製作所 ライフ事業統括本部 CSO）
瀧川 仁　（高エネルギー加速器研究機構 物質構造科学研究所 協力研究員）

分子科学研究所

渡辺 芳人 所長
山本 浩史 教授　（研究総主幹，装置開発室長）

4. 議論内容：

人事制度改革案について
電気代の高騰について（情報共有）

7-2　光分子科学研究領域の評価

7-2-1　Matthias Weidemüller 外国人運営顧問

Report on the visit to the Institute for Molecular Science (IMS), Okazaki

22 March to 27 March 2023

Matthias Weidemüller (Heidelberg University)

This report is based on a visit to the Institute for Molecular Science from 22 March to 27 March 2023. On 22 March, Director General Professor Watanabe gave a general overview of IMS. On 23 and 24 March, there were presentations by a selection of PIs from different research departments of the institute, namely Professors Ohmori, Kera, Katho, Y. Taira, Matsui, and Tanaka from the Department of Photo-Molecular Science, Professor Sugimoto from the Department of Materials Molecular Science, Professor Kuramochi from the Research Center of Integrative Molecular Systems, Professors Okamoto and Kumagai from the Center for Mesoscopic Sciences, and Professor Taira from the Division of Research Innovation and Collaboration. The presentations were about 40–50 minutes each, including discussion. In addition, after the general introduction into the scientific activities at UVSOR Synchrotron Facility by Professor Kera on 24 March, I was also given a tour of the facility by him on the next day. On 27 March, DG Professor Watanabe had a closing discussion with me. Additional information for this report was extracted from the Annual Reviews of IMS of the years 2021 and 2022.

First of all, I would like to thank all members of IMS participating in the review as well as the team organizing my visit, who made it such a rewarding experience for me. I greatly enjoyed high quality of the presentations as well as the openness and honesty in the scientific discussions. Despite the limited duration of my stay, I could get a very good impression on part of the scientific activities at IMS as well as its general structure, which I will describe in detail in the following.

Before starting, I would like to make two disclaimers. First, most of the topics presented during my stay do not fall into my specific area of expertise. Therefore, my assessment is based on a rather general scientific point-of-view and thus cannot be regarded as a thorough evaluation, but more as a first impression from a non-expert in the field. Second, I have a long-standing and very fruitful collaboration with Professor Ohmori. So far, we have published two joint papers in the last years, a third one is close to completion. Therefore, my view on his scientific work is positively biased, and this obvious conflict of interest should be taken into consideration with regard to my statements on his research activities.

General remarks

IMS is one of five National Institutes of Natural Sciences of Japan. It is involved in a large number of prestigious national science programs. With UVSOR, it hosts one of Japan's synchrotrons as a user facility specifically dedicated to study the structure and dynamics of chemical and condensed-matter systems. IMS maintains a large number of national and international collaborations. The training of graduate students is structured in the framework of the SOKENDAI Graduate University of Advanced Studies.

IMS meets highest international standards in terms of its scientific activities as well as its infrastructure. It hosts a large number of internationally highly renowned research groups acting at the forefront of modern science. Collaboration within the institute as well as with national and international partners appears to be natural, if not essential as part of IMS' mission and is supported by its structure through, *e.g.*, dedicated funds for joint research, inter-university research networks, or support for users at the multiple beamlines at UVSOR serving different research communities.

From the presentations and the discussions with the researchers from the various departments, I gained the very positive, general impression that their research is not merely driven by scientific mainstream or rather short-term goals, but instead by a deep interest in science as well as genuine curiosity. By the same token, technological developments are motivated by providing the best possible and sustainable solution to a given scientific question, be it, *e.g.*, instrumentation and detectors at UVSOR beamlines, or cutting-edge light sources in different IMS labs. Thus, these devices bear the promise to offer best performance and deliver excellent experimental results, thus setting standards for an entire field of research. I am certain that this kind of scientific honesty, paired with the serious dedication to the development of the best possible scientific instruments, is one of the key factors for IMS' outstanding national and international reputation.

UVSOR Synchrotron Facility and associated research groups

From the various presentations and the guided tour around UVSOR I came to the conclusion that such a facility is well suited to an institute of the size of IMS, as it can still be largely operated and maintained with local resources. The integration of the user facility into a diverse, inspiring scientific environment as represented by the different departments at IMS provides an important added value, which might even be explored further as it possibly was already in the past. UVSOR's operation parameters cover the range of comparably low energies (sub-GeV) combined with very high emittance. I am not an expert in electron synchrotron facilities at all, but all researchers involved in UVSOR could make a convincing case that the synchrotron is well positioned in the landscape of different synchrotron facilities in Japan and worldwide with regard to brightness and photon energies. Some of the experiments and investigations, in particular those addressing material science and biological applications, can actually be performed exclusively at UVSOR, also making use of its exquisite detector infrastructure. Therefore, UVSOR and its 14 beamlines serve a large number of national and, to a smaller extent, international users.

The different beamlines contain a large number of outermost sophisticated detectors serving a broad variety of scientific applications. Novel developments include tunable gamma-ray creation, generation of exotic light beams, and the development of Photoelectron Momentum Microscopy (PMM) and spin-resolved photoelectron spectroscopy. Due to the exquisite instrumentation, the beamlines cover a broad range of scientific applications ranging from condensed matter science, material science and biology, but also some more exotic topics such as medical applications or the structure analysis of meteorites.

Planning for future upgrade to the next generation of synchrotron facility at IMS, coined UVSOR IV, is already in progress. In this context, it will be an important task to provide a clear vision on how this future facility will maintain its competitive status, and to identify key scientific areas where the upgraded facility would provide unique scientific insights and world-leading discoveries. Ideally, design parameters for the facility as well construction plans for its instrumentation and detectors would follow from such general considerations.

Masahiro KATOH

Masahiro Katoh is responsible for the technological development and characterization of novel and highquality light sources at UVSOR. Important recent developments include the production of light beams with non-standard propagation properties (vortex and vector beams as well as temporally-structured light) using a combination of two undulators with a synchronized laser beam. In addition, a gamma-ray source based on laser-aided Compton scattering was developed offering tunable monochromatic gamma rays. A rather spectacular result is the detection of synchrotron radiation emitted from a single stored electron and the analysis of the corresponding detection statistics. Besides these scientific studies, he pushes technological design studies for the futures UVSOR-IV facility forward.

Fumihiko MATSUI

Fumihiko Matsui leads the development of photoelectron detectors at UVSOR for high-resolution electron and spin spectroscopy. He can look back to an impressive track record in the realization of 2D photoelectron spectrometers based on projection type analyzers for the study of spatially resolved atomic and electronic structure. Currently, he is heading towards further extending this technology to also reveal spin textures in condensed matter materials. While the focus of his work is on the development of instrumentation, there are important scientific results demonstrating, on the one side, the capabilities of the novel detectors. On the other side, serving the use of these detectors for studies of interesting properties of solid-state materials like, e.g., the valence band of graphite or chiral charge density waves. Being positioned between basic and applied science, his group maintains collaborations with scientific users of UVSOR from different academic institutions as well as with companies. His future plans follow a clear strategy and are well embedded into the general strategy of UVSOR. The outcomes of his activities are not only published as scientific papers, but there are also patents emerging from the technological developments.

Kiyohisa TANAKA

The group of Kiyohisa Tanaka develops instruments for Angular-Resolved Photoelectron Spectroscopy (ARPES) and applies these instruments to the investigation of the electronic structure of high-T_c superconductors, in particular from the families of cuprates and ironpnictides. For the cuprates, the role of phonons for the enhancement of the transition temperature could be revealed, while for the ironpnictides, the superconducting gap could be observed in the electronic structure of a specific material. His scientific program is well balanced between questions from basic condensed-matter science and the required technological development of instrumentation for addressing these questions. The latest technological achievements comprise the development of a new highly efficient spin resolved ARPES system with drastically improved momentum and energy resolution. Soon, information on the spin structure will be accessible in all three dimensions by the integration of a spin manipulator foreseen as the next upgrade of the instrument.

Yoshitaka TAIRA

The research theme of Yoshitaka Taira is the the generation of novel gamma-ray sources using high-energy electron beams. He uses the unique possibilities offered by UVSOR's energy range to create cw or pulsed gamma rays in the mid-MeV range through inverse Compton scattering. As an important application, the availability of coherent gamma radiation at UVSOR opens novel applications using positron annihilation spectroscopy for probing defects in condensed matter samples. As a specific innovation, age-momentum correlations have recently been demonstrated successfully as an extension of standard positron annihilation spectroscopy. Future plans include the generation of spin-polarized positrons using the available circularly polarized gamma rays, and the creation of gamma-ray vortex beams from Nonlinear Inverse Thomson Scattering based on a proposal of Professor Taira and coworkers. Professor Taira recently joined IMS. His research is very well embedded into the research agenda of UVSOR facility, significantly extending the current capabilities of gamma-ray generation and offering intriguing applications in material research through high-resolution gamma-ray induced positron annihilation spectroscopy.

Research groups from the Department of Photo-Molecular Science

Kenji OHMORI

The group of Kenji Ohmori pursues non-standard approaches for the implementation of quantum information processing and quantum simulation. The experiments ingeniously combine techniques from the physics of ultracold gases, in particular Bose-Einstein condensates, optical lattices, optical tweezers and frozen Rydberg gases, with the application of coherent control techniques employing ultrashort laser pulses. As a recent highlight, the group has demonstrated controlled energy exchange between two single Rydberg atoms on a nanosecond time scale, which constitutes an important precursor step for implementing ultrafast qubit gates. Kenji Ohmori is internationally highly recognized and plays a leading role in Japan’s national quantum information program. His group is internationally highly connected and recognized, which is also reflected by the large number of highly talented international researchers and PhD students working in his team.

Hiromi OKAMOTO

Hiromi Okamoto is an internationally highly renowned researcher famous for his contributions to near-field chiro-optical imaging and microscopy. The work which he presented in our meeting was truly impressive. Among recent spectacular results are, the observation of the enhancement of spin–orbit interactions and chirality by a pair of oppositely polarized spins in an organic chiral superconductor, the development of high-precision circular dichroism spectroscopy, or the demonstration of optical gradient forces on chiral particles. These achievements provide exciting perspectives for further future developments in the field of nanoscopic chiroptics with plasmonic enhancement. Without any doubt, he will continue to shape this important research field as one of its internationally leading researchers.

Satoshi KERA

Satoshi Kera fulfills a double task at IMS in an impressively effective manner: On the one hand he is the head of the UVSOR facilities and thus responsible also for developing concepts for the next upgrade of this synchrotron facility (see statements on USVOR above). On the other hand, he also leads a research team devoted to studies of the electronic properties of functional organic materials. While his core group is rather small with only few students, he takes great profit from collaborations with researchers exploring the rich capabilities of the UVSOR facility and its dedicated beam lines, like, *e.g.*, the Photoelectron Momentum Microscope. One current focus of his research are studies on the dynamics of polaron formation and dynamics in organic semiconductor materials.

Research group from the Department of Materials Molecular Science

Toshiki SUGIMOTO

Toshiki Sugimoto and his team study the role of interfacial water and ice using heterodyne-detected nonlinear spectroscopy for unveiling the molecular orientation. This innovative technique, which directly detects the proton configuration of the OH-stretching mode in water molecules, finds fruitful applications in a broad variety of material systems as explored by his group at IMS. Recent achievements include the observation of the emergence and disappearance of net proton order in heteroepitaxially grown crystalline ice films on metal surfaces as a model system of a strongly correlated proton system, or the impact of interfacial water on the C–H activation in photocatalytic methane conversion. Overall, Toshiki Sugimoto makes very efficient use of the unique capabilities of the nonlinear spectroscopy methods, which he developed, to a broad range of systems featuring interfacial water. The results obtained have high impact on the fundamental understanding of the importance of interfacial water as well as offering intriguing opportunities for engineering surfaces for novel functionalities in water aggregates.

Research group from the Research Center of Integrative Molecular Systems

Hikaru KURAMOCHI

Hikaru Kuramochi has recently joined IMS faculty from RIKEN introducing advanced ultrafast spectroscopy for studies of chemical reaction dynamics reaching from larger molecular ensembles down to the single-molecule level. For this purpose, the group also develops novel light sources for highly sensitive time-resolved 2D Raman spectroscopy of electronic and vibrational molecular degrees of freedom. In the past, Hikaru Kuramochi has already obtained impressive scientific results with high impact. Based on his outstanding career path, he presented a very ambitious, yet convincing work program with thetrealistic perspective to produce important scientific results at IMS in the very near future. Within a very short period of time, the (still rather small) group has build up a state-of-the-art laser lab featuring Raman spectrometers with unprecedented performance and has already realized the essential precursor steps for single-molecule ultrafast spectroscopy. I was intrigued by the nice combination of cutting-edge technological developments with exciting applications to basic science. The group maintains collaborations with a large number of groups in Japan, in particular for exploring a broad variety of molecular and material systems using the unique capabilities of time-resolved Raman spectroscopy. The future prospect of applying time resolved correlation spectroscopy to single-molecular complexes in solution could potentially become a real game-changer for the entire field of molecular reaction dynamics.

Research group from the Center for Mesoscopic Sciences

Takahashi KUMAGAI

Takahashi Kumagai recently came to IMS starting a new field of research on atomic-scale optical microscopy based on his previous experience as research group leader at the Fritz-Haber Institute in Berlin. He combines enhanced near-field optical coupling at specially designed plasmonic tips near surfaces with quantum plasmonics in the STM junction and time resolved femtosecond laser spectroscopy. In a series of spectacular experiments, he could reach sensitivity down to the single atom or molecule level. At IMS, he is now further developing this intriguing field of research by combining ultra broadband pulsed laser sources with atomic-force microscopy. In a very short period of time, he has set up a world-class lab at IMS. His ambitious goals already bear first spectacular results on nanoscale mid-infrared imaging and single-protein infrared spectroscopy. His group maintains a large number of national and international cooperations. I was very impressed not only by the internationally highly competitive research program, which he presented, but also by the outstanding results already achieved at IMS.

Research group from the Division of Research Innovation and Collaboration

Takunori TAIRA

Takunori Taira holds a double appointment at IMS and RIKEN. His expertise is on the development of laser ceramics for the realization of high-power laser sources, coined TILA (Tiny Integrated Laser). These ceramics laser materials find a broad variety of applications ranging from laser-driven beam accelerators over narrowband Terahertz generation and material processing to microlaser-induced ignition of combustion engines. Professor Taira has formed a large consortium of academic institutions and companies to further promote the TILA technology and to explore novel applications. For this purpose, a dedicated TILA Laboratory has been established at IMS. The excellent activities of Professor Taira demonstrate the remarkable potential of combining basic research with technological progress at IMS.

In conclusion, IMS hosts a large number of outstanding scientific groups covering a broad range of fields, yet with a tangible general mission in fostering interdisciplinary research in the crossroads between physics, chemistry and material science. I gained an outermost positive impression of its scientific and technological excellence, which makes it one of Japan's internationally highly visible research centers. My visit was very enjoyable from a professional as well as personal perspective, and I would like to thank all participating members of IMS for great efforts and their warm hospitality.

Heidelberg, 30 April 2023

7-3　生命・錯体分子科学研究領域の評価

7-3-1　David A. Leigh 外国人運営顧問

Prof. Dr. Yoshihito Watanabe

Director General

Institute for Molecular Science

Okazaki

Japan

24th April 2023

Dear Director Watanabe,

Evaluation of the Department of Life and Coordination-Complex Molecular Science
of the NINS Institute for Molecular Science, Okazaki, Japan

Many thanks for the warm and kind hospitality of you and your colleagues during my on-site visit to the NINS Institute for Molecular Science on 6–8 March 2023. During my visit I was given in-depth presentations by Prof. Ryota Iino, Director of the Department of Life and Coordination-Complex Molecular Science, and other members of the Department and IMS. I also received presentations from Prof. Masahiro Ehara, Director of the Research Center for Computational Science (RCCS), Prof. Satoshi Kera, Director of the UVSOR Synchrotron Facility, Prof. Koichi Kato, Ex-Director of the Exploratory Research Center on Life and Living Systems (ExCELLS) and Distinguished Professor Makoto Fujita of the Division of Advanced Molecular Science. For reasons of clarity I have organised my report in 4 Sections, plus a Summary at the beginning.

Summary

The Department of Life and Coordination-Complex Molecular Science at IMS is a center of research excellence that is tackling some of the most important and profound challenges in the molecular sciences today. Its success and performance is reflected not only in the outstanding research outputs (in terms of journal publications, invited lectures and prizes) of the current PIs, but also in the remarkable number of high quality scientists that have started their independent careers at IMS and then moved to be highly successful Associate or Full Professors at other universities.

The Institute and Department strengths include that the staff are well motivated and perform at the highest level. The leadership is outstanding. The level of equipment and instrumentation is well above that of many world class laboratories in the USA and Europe. This gives the groups at IMS a significant advantage over competitors worldwide in terms of their ability to tackle the toughest problems in science today. However, the IMS groups are considerably smaller than those of international competitors, which means that they simply do not have the human resource to exploit breakthroughs as quickly or as well as larger competitor groups internationally. A contributing reason for the small group sizes is the available budget for personnel, which is perhaps half that of competitors in the USA and Europe. Another factor may be poor access to the best students for recruitment purposes because of a general lack of integration and cooperation for mutual benefit with universities. A striking weakness in terms of staffing is the lack of diversity in gender at PI level. In my opinion, it is important for IMS, and for the future of Japanese science in general, that this is addressed as quickly as possible.

1. Overall impressions

My overall impression of IMS, and the Department of Life and Coordination-Complex Molecular Science in particular (one of the four Departments of IMS), is over-whelmingly positive: It is an influential and highly respected institute in the field of the molecular sciences. The Department of Life and Coordination-Complex Molecular Science is globally renowned for carrying out high quality innovative research, its strong faculty, an excellent research environment, and collaborations with other institutions and universities, all of which make it a leading centre for research internationally.

2. The role of IMS in the national scientific landscape

The Institute for Molecular Science was founded in 1975. I believe that one reason for establishing national research institutes at that time was to support and supplement the national research effort of universities by being a focal point for 'big' facilities that individual universities could neither afford to purchase nor to run. This remains a compelling need today, for example few universities would be able to run a synchrotron. Nevertheless, the scientific era we live in now is very different from the 1970s, and many universities have large instruments and facilities that serve as resources for others researchers in Japan and worldwide. Within this changing scientific climate, research institutions and their position in national and international science strategies benefit from growth and revaluation of purpose. In particular, the role and interaction of research institutions with other national bodies, such as universities, should evolve. In this regard, I note that IMS has undergone a healthy number of changes in structural organisation over its lifetime, including the establishment of many new, highly successful and internationally important, research centers.

A key part of IMS's Mission Statement is that it should '…*enhance the progress of molecular science covering broader research areas via mutual exchange of human resources among all the universities in this country*…'. IMS fulfils this role admirably by providing an opportunity for researchers to be fully independent at a much earlier stage (associate professor) than is traditional in Japanese universities. For a dramatic example of the impact that independence at a young age can have in the chemical sciences, one need look no further than the 2021 Nobel Prize in Chemistry, awarded to Ben List and David MacMillan for the development of asymmetric organocatalysis. The two seminal papers that led to that Nobel Prize were the first (List) and second (MacMillan) papers of the recipients as independent PIs. Perhaps because they have no scientific program of their own to build on initially—or perhaps because of the impetuosity of youth(!)—young PIs are often less conservative than more established PIs and more inclined to explore radically new concepts and ideas that can lead to breakthroughs, and even completely new fields of science. The consequences of this aspect of IMS's employment policy must be taken into account in any objective consideration of the impact and success of IMS.

Since IMS was founded in 1975, more than 60 IMS associate professors have been promoted to full professors or similar positions at other institutions, including the following researchers who are particularly relevant to the research area covered by the Department of Life and Coordination-Complex Molecular Science: Tatsuya Tukuda (Professor, University of Tokyo; https://www.chem.s.u-tokyo.ac.jp/users/chemreact/index-e.html); Takeaki Ozawa (Professor, University of Tokyo; https://analyt.chem.s.u-tokyo.ac.jp/en/); Hirokazu Tada (Professor, Osaka University; http://molectronics.jp/en/); Hidehiro Sakurai (Professor, Osaka University; https://www-chem.eng.osaka-u.ac.jp/~sakurai-lab/en/index.html); Donglin Jiang (Professor, National University of Singapore; https://blog.nus.edu.sg/chmjd/professor/); and Shigeyuki Masaoka (Professor, Osaka University; http://www.chem.eng.osaka-u.ac.jp/masaoka_lab/english/index.html).

In addition, nearly 130 IMS assistant professors have been promoted to full professors or similar positions at other institutions. Outstanding examples include: Mitsuhiko Shionoya (Professor, University of Tokyo; https://www.chem.s.u-tokyo.ac.jp/~bioinorg/indexE.html); Hiroshi Kitagawa (Professor, Kyoto University; http://kuchem.kyoto-u.ac.jp/ossc/index.html); and Hajime Ito (Professor, Hokkaido University; https://itogrouphp.eng.hokudai.ac.jp/).

These are staggeringly successful numbers. Although Japanese universities are increasingly allowing full independence of PIs earlier in careers, I believe that this is still one of the most important factors that makes IMS stand out as an attractive institution for outstanding young researchers wanting to start their independent academic career.

However, the very success of this role of IMS disadvantages the institute in terms of metrics such as citations and international awards. Since promotions in IMS are prohibited, all of your (very successful) young staff have to leave to be promoted elsewhere. It is at the Full Professor stage that one gets the full benefit, in terms of citations, recognition and funding, of having built an internationally important research program. The tremendous success of IMS is thus reflected in these 190(!) staff that have been promoted to positions elsewhere in the 48 years since it was founded. That is, on average, nearly 4 staff members a year for an institution that currently numbers 36 Full, Associate and Project Professors and 40–50 Assistant Professors.

3. Gender imbalance and lack of international diversity at PI level

IMS currently has 18 Full Professors (including Distinguished Professor Fujita), 16 Associate Professors and 2 Project Professors. Of these 36 senior academic staff, just one (Assoc. Prof. Momiyama) is female. This extremely poor gender imbalance at PI level is a weakness for many reasons: First of all it means that IMS is missing out on a huge amount of talent; secondly, it means there is a lack of senior role-models in IMS that would showcase to female young researchers that IMS is well set up for women to succeed in a scientific career. In contrast, the junior positions (PhD and Post-Doctoral Fellows) in all of the research groups I met with had good gender balance (typically 30–50% female). There are no doubt many reasons—historical, cultural, social and practical—that contribute to the gender imbalance at PI level, but it is a problem that I strongly suggest you start solving immediately.

Of course, it would be wrong to suggest that IMS is unique in having a gender imbalance problem; my own Department has only 15 women PIs out of 80 faculty, which is probably typical of UK Chemistry Departments. It is an issue in science academia that many western countries struggled with. My advice is to start by asking female professors and female PhD students what they think are the issues involved and what would make a difference to them. Then it will be up to men and senior leadership to take the lead in implementing solutions that women feel would make a difference. If, for example, young women scientists tell you that the non-promotion of Assistant or Associate Professors within the Institute is an issue because it is desirable to have stable roots for starting or growing a family then, in my view, that rule should be *very publicly* removed for women scientists. Other ways of supporting women professors, such as giving them a PDRA for a year any time they give birth to help them run their group during this important time, should be considered if, again, young female scientists tell you that they are reluctant to pursue academic careers because of the difficulty of juggling a young family with establishing their research program. These are examples of the sort of initiatives that might help make IMS an institute that women PIs really want to join. Let me reiterate that in my opinion the role of men in this should be to put into place initiatives that women say they want; it is not for men to concoct plans that they *think* women want.

Also on the issue of diversity, although less important, it feels to me like a missed opportunity that all 36 of the professors in IMS are Japanese. There is some international diversity within research groups—Prof. Iino's group is an excellent example of this—it is at PI level that it is lacking. As with gender, diversity in terms of origins, ethnicity, upbringing and education brings different ways of thinking, not just with regards as to how to tackle scientific problems, but also in the way institutes and laboratories are organised and run. Europeans and Americans love Japan: The people, the culture, the country and the food. Although there may be cultural and language issues with attracting outstanding foreign PIs of the quality that would benefit the institute to move full time to Japan, I suggest it would be easy for IMS to attract outstanding foreign PIs to have satellite labs at IMS. Many leading chemists (including Fraser Stoddart, Ben Feringa and myself in the molecular machines field) have satellite labs in China, for example. I believe the Chinese have found that our presence (and that of many others) gives them insight into how leading US and UK scientists think and run their research programs and labs and that has benefitted Chinese science in their ways of thinking and scientific culture. Perhaps this is something that IMS could consider, maybe through participating in or leading bids in the WPI program, which could provide funding for such cross-national appointments.

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

The Department has 8 research groups, four primarily associated with studies on the molecular basis and mechanisms of biological systems (Iino, Kato, Aono and Nakamura) and four motivated by unsolved problems in chemical synthesis (Uozumi, Kusamoto, Momiyama and Segawa). All of these groups are of very high quality; they tackle important fundamental problems in creative ways and publish their findings in the best international journals.

Prof. Ryota IINO

Professor Iino's research focuses on the study of biomolecular motors using advanced imaging techniques. He is a world leader in the use of super-resolution microscopy to investigate the operational and design principles of molecular motors. These include the visualisation of fast dynamics of motor-molecules such as V-ATPase, kinesin, chitinase and dynein by single-molecule imaging. In the last few years he has expanded his group's program to include the development of new cutting-edge single-molecule techniques for angstrom-precision tracking and high-speed tracking. This is a highly competitive area trying to answer profound questions regarding the way that biology works at the molecular level. Recent highlights include "*Direct observation of stepping rotation of V-ATPase reveals rigid component in coupling between V_o and V_1 motors*," *Proc. Natl. Acad. Sci. USA* **119**, e2210204119 (2022) and "*Combined approach to engineer a highly active mutant of processive chitinase hydrolyzing crystalline chitin*," *ACS Omega* **5**, 26807–26816 (2020).

Prof. Yasuhiro UOZUMI

Professor Uozumi is a highly respected international leader in the development of highly effective heterogeneous catalysts, particularly for applications in green chemistry. In recent years he has developed highly active ppb-catalysts with turnover numbers >3 million for various coupling reactions and developed polymer supported asymmetric Pd-catalysts that work in water. He has recently applied his expertise in polymer supported reagents to photoredox catalysis in water, bringing a 'green' perspective to one of the hottest areas of synthetic organic chemistry today. Recent highlights include "*Photocatalytic carbinol cation/anion Umpolung: Direct addition of aromatic aldehydes and ketones to carbon dioxide*," *Org. Lett.* **23**, 7194–7198 (2021) and "*Production of bio hydrofined diesel,* *jet fuel, and carbon monoxide from fatty acids using a silicon nanowire array-supported rhodium nanoparticle catalyst under microwave conditions*," *ACS Catal.* **10**, 2148–2156 (2020).

Assoc. Prof. Norie MOMIYAMA

Associate Professor Momiyama is well known for her significant, original and important contributions in asymmetric organocatalysis. She continues to use halogen bonding as a recognition element in new organocatalysts and polymer catalysts. She has recently started a highly ambitious program on the digitisation of chemistry which seeks to take organic synthesis to the frontiers of what is chemically possible. Recent highlights include "*Three-center-four-electron halogen bond enables non-metallic complex catalysis for Mukaiyama–Mannich-type reaction*," *iScience* **25**, 105220 (2022) and "*Chiral counteranion-directed catalytic asymmetric methylene migration reaction of ene-aldimines*," *J. Org. Chem.* **87**, 9399–9407 (2022).

Assoc. Prof. Tetsuro KUSAMOTO

Associate Professor Kusamoto's group create photofunctions based on stable radicals. These include luminescent systems based on photostable triaryl radicals and magnetoluminiscent systems. His group have a series of papers in the top journals in the field, such as *JACS* and *Angewandte Chemie*. Recent highlights include "*An open-shell, luminescent, two-dimensional coordination polymer with a honeycomb lattice and triangular organic radical*," *J. Am. Chem. Soc.* **143**, 4329–4338 (2021) and "*Radical-based coordination polymers as a platform for magnetoluminescence*," *J. Am. Chem. Soc.* **143**, 5610–5615 (2021).

Assoc. Prof. Yasutomo SEGAWA

Associate Professor Segawa is widely regarded internationally as a rising star in the field of organic chemistry. His research focuses on the development of new synthetic methods and strategies for constructing topologically complex carbon-rich molecules. He has published the synthesis of a series of extraordinary catenanes and knots and Mobius strip molecules. His research achievements have been published in the highest impact, most visible, journals, including *Science*, *Nat. Chem.*, *Nat. Synth.*, *JACS* and *Chem*. Recent highlights include "*Synthesis of a Möbius carbon nanobelt*," *Nat. Synth.* **1**, 535–541 (2022) and "*Topological molecular nanocarbons: All-benzene catenane and trefoil knot*," *Science* **365**, 272–276 (2019). In addition, he has started a research program on microcrystal electron diffraction structure determination which offers the potential for revolutionising structure determination of organic molecules.

Assoc. Prof. Akihiko NAKAMURA (cross-appointment)

Associate Professor Nakamura is a cross-appointment with Shizuoka University and his group's research interests include protein engineering, heterogeneous enzyme catalysis, and single-molecule analysis. His research program is involved in developing and improving plastic degrading enzymes which have the potential to solve critical environmental problems related to plastic degradation. Recent highlights include "*Positive charge introduction on the surface of thermostabilized PET hydrolase facilitates PET binding and degradation*," *ACS Catal.* **11**, 8550–8564 (2021) and "*Domain architecture divergence leads to functional divergence in binding and catalytic domains of bacterial and fungal cellobiohydrolases*," *J. Biol. Chem.* **295**, 14606–14617 (2020).

Prof. Koichi KATO (ex-Director of ExCELLS)

The ambitious aims of this group are to understand how chemistry becomes biology, the origin of life. This is one of the contemporary 'Grand Challenges' of science, involving chemistry, physics and biology. Professor Kato collaborates with many groups around the world and has been hugely successful in establishing major consortia, such as ExCELLS. His group's own research program is aimed at answering fundamental questions such as what is the blue print for protein glycosylation? and what are the design principles for protein assembling systems? Recent highlights include "*Key residue for aggregation of amyloid-β peptides*," *ACS Chem. Neurosci.* **22**, 3139–3151 (2022) and "*An embeddable molecular code for Lewis X modification through interaction with fucosyltransferase 9*," *Commun. Biol.* **5**, 676 (2022).

Prof. Shigetoshi AONO

Professor Aono is a bioorganic chemist whose research interests revolve around metalloproteins and sensor proteins. His group are working to establish the protein machinery responsible for the active site assembly and maturation of NiFe-hydrogenases and also the molecular mechanism of O_2 sensing and signal transduction by the HemAT/CheA/CheW complex. Recent highlights include "*Crystal structural analysis of aldoxime dehydratase from Bacillus sp. OxB-1: Importance of surface residues in optimization for crystallization*," *J. Inorg. Biochem.* 230 (2022) and "*Heme controls the structural rearrangement of its sensor protein mediating the hemolytic bacterial survival*," *Commun. Biol.* **4**, 467 (2021).

There are a number of successful collaborations between groups in the Department of Life and Coordination-Complex Molecular Science and other groups in IMS that clearly add value: For example, the Uozumi group with Prof. Ehara (Dept. Theoretical Comp. Mol. Sci.); Prof. Momiyama working with Prof. Suzuki (Instrument Center) on the design and understanding of complex catalysts; a series of highly successful collaborations between the Iino group and Prof. Okazaki (Dept. Theoretical Comp. Mol. Sci.) on simulations of chitinase, with Prof. Koga (ExCELLS) and Kosugi (CIMoS) on computational engineering of PET hydrolase and redesigning of V_1-ATPase, and with Profs. Kumagai and Nishida (Mesoscopic) on single protein vibrational spectroscopy; as well as a series of collaborations between the Kato group and various groups that bring both experiment and theory to bear on problems relating to amyloid formation mechanisms.

The quality of equipment in each group's laboratories in the Department of Life and Coordination-Complex Molecular Science, and in the institute in general, is outstanding and significantly better than almost all university laboratories worldwide. The Segawa laboratories, in particular, are one of the best equipped labs for cutting-edge organic synthesis that I have ever seen. They are better equipped than my own lab, which is one of the best equipped labs in the UK! This gives the groups at IMS a significant advantage over competitors worldwide in terms of their ability to tackle the toughest problems in the molecular sciences today.

However, although they are highly productive, the groups tend to be significantly smaller than that of their international competitors (my own group, for example, is 30–35 researchers, equally split between PhD students and postdoctoral scientists). The small size of the groups in the Department inevitably means that they do not have the person-power necessary to capitalise on conceptual breakthroughs as quickly as others around the world would do.

I think that there are several ways that IMS could consider addressing this issue:

(i) The first is that, in my opinion, there needs to be an increase in budget. I realise that it is always easy to say ‘give more money’ but, in this case, it is clear that the groups are underfunded in terms of personnel by a factor of 2 compared to their international competitors. This is a key disadvantage when one is in competition to find answers to important scientific problems.

(ii) A second approach that might be useful could be to reconsider your relationship with universities. As I noted earlier, you have more and better laboratory equipment than universities, but they have more—and better access to—young researchers in the form of students. I suggest you consider the possibility of having more cross-appointments with universities, perhaps having IMS staff teach courses at the universities (which would give potential PhD students exposure to IMS staff as well as easing teaching loads for staff at universities). In this way universities would benefit by having easier access to more equipment and extra staff who would teach, while IMS would benefit from having better access to a larger pool of potential researchers. However, if this is done, care must be taken to ensure that cross-appointments are done properly. If I recall correctly, the cross-appointment of Prof. Nakamura requires him to teach a full teaching load at Shizuoka University. That appears from the outside to be completely inappropriate; if it is a cross-appointment then I would expect half his salary should be paid by the university (and half by IMS) and he should have, at most, a 50% teaching load and no administration at the university so as to take into account all the additional travel and work he has to do in order to play a substantial role in two locations.

I hope that this short report proves useful to you and your colleagues in thinking about how to continue to develop IMS. It is a truly fantastic institute with excellent scientists doing world class research. It has been a pleasure to visit and interact with such inspiring people, from the young researchers to the thoughtful generous leadership. Thank you for this opportunity.

Best wishes,

David A. Leigh FRS
Royal Society Research Professor & Sir Samuel Hall Chair of Chemistry, University of Manchester, UK
24 April 2023