# 5．点検評価と課題

2022 年 4 月から研究顧問をお引き受けいただいている James M. Lisy 教授（イリノイ大学）と北川　進教授（京都大学），産学連携研究アドバイザーに就任いただいている菊池　昇博士（(株) トヨタコンポン研究所所長）と福田伸博士（(株) 三井化学分析センター技術顧問）に 2024 年 5 月開催の IMS Presentations 2024 に現地参加頂き，所全体の研究評価，研究体制，産業界の視点からの研究評価などについての提言をいただいた。

独マックスプランク高分子研究所 Mischa Bonn 教授と英オックスフォード大学 David Manolopoulos 教授が 2024 年 10 月に来所し，それぞれ物質分子科学研究領域と機器センタ，理論・計算分子科学研究領域と計算科学研究センターを中心にヒアリングが実施され，各グループの研究内容やセンターの活動を評価いただいた。加えて，分子科学研究所の全般的な課題について所長と議論した。

（渡辺芳人）

## 5-1　研究顧問／産学連携研究アドバイザーによる点検評価

分子科学研究所では，法人化の前から所長が研究面を諮問するために研究顧問制度を導入している。第一期中期計画期間では国内 3 名の研究顧問が，所内の各研究グループによる予算申請ヒアリングに参加し，それぞれについて採点し，所長はその採点結果を参照しつつ各研究グループに配分する研究費を決定してきた。第二期中期計画期間は国際的な研究機関としての研究面を中心に諮問することとし，国外委員も追加することとした。第三期中期計画期間から国内外各 1 名で運用している。これに加えて第四期中期計画期間（2022 年度～ 2027 年度）より，分子科学の分野において特に優れた研究業績を有する者又は 産学連携関係に特に精通した者に, 研究所の産学連携研究に関する指導，助言等をお願いする「産学連携研究アドバイザー」を新たに設けた。産業界で研究所長などの責を担っているアドバイザーから見て，基礎研究が中心となっている分子科学研究所の個々の研究者の研究課題や成果がどのように受け止められるのかをフィードバックして頂くた めの制度である。また，アドバイザーが有するネットワークを通じて，分子科学研究所の研究が産業界に広く知られることも期待するものである。 産学連携研究アドバイザーには，予算申請ヒアリング（2024 年 5 月 9–10 日開催）に同席して頂き，評価の過程に加わって頂くと共に，社会実装や産業利用に資する可能性のある研究成果の発掘をお願いしている。その結果として，企業による分子研各施設の利用や研究者間の交流が始まっている。

研究顧問（2024 年度）

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| 北川　進 | 京都大学副学長，特別教授 |
| LISY, James M. | Research Professor, University of Illinois Urbana-Champaign |

産学連携研究アドバイザー（2024 年度）

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| 菊池　昇 | 株式会社トヨタコンポン研究所代表取締役所長 |
| 福田　伸 | 株式会社三井化学分析センター技術顧問 |

## 5-2　理論・計算分子科学研究領域の評価

### 5-2-1　David E. Manolopoulos 外国人運営顧問

**Report on first visit to IMS, 1–4 October 2024**

1. Scientific discussions with members of the IMS faculty

**Prof. Hiroshi Yamamoto**

I had a very interesting discussion with Prof. Yamamoto about his work on chirality and the CISS (chirality induced spin selectivity) effect, in which he showed me the results of his experiment revealing giant spin polarisation in a chiral superconductor. Prof. Yamamoto was one of the first to become interested in the CISS effect as a result of a visit to IMS by Ron Naaman, and the experiments he has since done on it are quite remarkable. He has found a spin polarisation of around 80% in the chiral superconducting device he has fabricated, which is comparable to the spin polarisation found in earlier work on photoelectron currents through DNA. Both effects are too large to be explained by any simple theory so a great deal of theoretical work is now being done to try to understand them. These experiments performed at IMS have therefore made a truly significant contribution to an exciting new field.

**Prof. Shinji Saito**

I first met Prof. Saito when he visited Oxford around five years ago, and I am of course well aware of his work as an Editor for the Journal of Chemical Physics (JCP), where he has published a number of very fine papers. It was therefore a pleasure to meet him again and to hear about his recent work on dynamic phenomena in condensed phase systems. He described how he has constructed an accurate Frenkel exciton model for the photosynthetic light harvesting complex LHCII and then presented a wonderfully detailed analysis of hydrogen bond dynamics in supercooled water. Both studies struck me as absolutely first rate. This is the best work that has been done on either of these problems to date.

**Prof. Masahiro Ehara**

Prof. Ehara is an expert in accurate (correlated) electronic structure theory and its application to interesting chemical problems. His more recent work has focussed on the development of new methodology and on the application of time-dependent density functional theory (TD-DFT) to the excited states of systems that are beyond the reach of correlated wavefunction techniques. He began by describing a new inverse design method he has developed to target specific properties of molecule-nanoparticle systems. He then described his recent applications of TD-DFT to problems ranging from the photoluminescence and conductivity of carbon and BN materials to the suitability of nanoclusters for heterogeneous catalysis. These are topical studies and they seemed to me to have been executed extremely well, at least in part because of Prof. Ehara’s expertise with more accurate techniques (TD-DFT is only safe in the hands of those who understand its limitations!).

**Associate Prof. Kei-ichi Okazaki**

Prof. Okazaki gave me a truly beautiful presentation about his work on biomolecular machines. He began by explaining how his group’s molecular dynamics simulations of the $F_1$ catalytic motor in ATP synthase had provided mechanistic insight into the ATP synthesis/proton pump reversal experiments performed by Dr. Kobayashi. The simulations were published along with the experimental data in *Nature Communications* in 2023 and they have since resulted in Dr. Kobayashi winning an early career award from the

Biophysical Society of Japan. Prof. Okazaki then went on to describe how his simulations of the "inward open" → "outward open" transition in a transmembrane transporter protein have led to an interesting prediction that is currently being tested by his experimental collaborators: When the wild type protein is put into alpha-fold the resulting folded structure is purely "outward open," whereas when a D280 mutant is put into alpha-fold it is purely "inward open." He also described how the use of "shallow multiple sequence alignment (MSA)" rather than the default optimisation setting in alpha-fold results in structures along the reaction path between "outward open" and "inward open," as can be verified by running molecular dynamics from these intermediate structures. This is an intriguing result that seems to open up the possibility of gaining mechanistic insight from alpha-fold optimisations. Prof. Okazaki ended his presentation by describing his coarse-grained simulations of membrane deformations induced by the protein Pacsin 1. These too were interesting: The standard cartoon is that the protein squeezes the membrane until it breaks but his simulations suggest that quite the opposite happens: The protein instead stretches the membrane locally resulting in narrower sections nearby, which are where the breaks then presumably occur. Indeed some recent high speed atomic force microscopy experiments seem to corroborate this. Needless to say I found Prof. Okazaki's presentation extremely impressive from beginning to end.

**Associate Prof. Hisashi Okumura**

Prof. Okumura's presentation was focussed on using molecular dynamics simulations to shed light on the important problem of amyloid-β (Aβ) peptide aggregation. He began by describing his atomistic molecular dynamics simulations of β-hairpin formation in Aβ40 and Aβ42 (a variant with two extra residues that is known to aggregate faster than Aβ40). These simulations found the Arg5 residue to form a hydrogen bond to one of the two additional residues in Aβ42, a prediction has since been supported by Arg5 mutation experiments performed by Prof. Kato. Hence Arg5 appears to be the key residue that explains the greater tendency of Aβ42 to form β-hairpins, which presumably also explains why it aggregates faster. To investigate this further, Prof. Okumura is now performing some very large-scale (32 peptide) molecular dynamics simulations of the aggregation kinetics of Aβ40 and Aβ42 in aqueous solution. While the preliminary results of these simulations look interesting, their statistical errors are still too large to draw any firm conclusions from, despite the fact that the calculations have already been running for 5 years. This is clearly because Prof. Okumura has chosen to do fully atomistic simulations, which require a great deal of computer time for such large systems. I would strongly encourage him to develop a cheaper coarse-grained model and use that instead. Coarse-grained models are not always as reliable as atomistic simulations, but with the atomistic simulations he has already done he has more than enough data to fit a coarse-grained model that should be good enough to capture the processes he is interested in at the thermodynamic state point he is studying, for example with the help of modern machine-learning techniques. I hope this suggestion helps and that by next year he will be in a position to show me some well-converged Aβ aggregation kinetics results.

**Prof. Akihito Ishizaki**

I have followed Prof. Ishizaki's research for a number of years and enjoyed meeting him and listening to his talks at conferences, so it was a real pleasure for me to end my meetings by hearing about his latest research interests. Prof. Ishizaki is a deep thinker who works on difficult problems. He outlined his preliminary attempts to go beyond the usual assumption of a Gaussian environment by considering a quantum system in the presence of Poisson noise, his work on entangled photons that suggests the possibility of a simpler alternative to four-wave mixing experiments, and his work on the use of network modelling to find the excitation energy transfer bottlenecks in the photosystem II super-complex. All of this work is profound and at the very forefront of modern condensed phase quantum dynamics. Prof. Ishizaki's move to Tokyo will be a serious blow to the IMS and I sincerely hope that the institute will be able to find someone of equal stature to fill his shoes.

### 2. Visits to IMS Facilities

Prof. Ehara kindly showed me the computer cluster at the Research Centre for Computational Science, and Prof. Matsui kindly gave me a guided tour of the UVSOR Synchrotron Facility. Both were thoroughly enjoyable. I found the UVSOR Facility especially interesting as I have never visited a synchrotron before. Prof. Matsui explained its operation to me extremely clearly and knowledgeably. His enthusiasm for the facility was delightful!

### 3. Discussion with the Director General

**Prof. Yoshihito Watanabe**

I began my visit with a meeting with the Director General, Prof. Watanabe. Much of our discussion focussed on retention and other difficulties associated with running the IMS in the current financial climate (the Yen has decreased in value by 35% against the dollar in the last three years so overheads are now exceptionally high), and on some of the initiatives he has put in place to overcome them. These include increased support for PIs in receipt of large research grants, the option for those with sufficient grant income to support their research to extend their retirement age from 65 to 70, and the idea of encouraging Associate Professors whose research activity has not enabled them to secure promotions at top tier universities to apply for promotions at provincial universities instead. All of these initiatives strike me as sensible and in line with what other institutions (including my own) are doing to remain competitive.
For example, Prof. Omori has recently secured a very significant grant for quantum computing, the overheads of which contribute 4% to the total budget of IMS. New "designated professorships" have been created with competitive salaries and a tenure of up to 10 years to enable him to recruit suitably qualified project leaders for this grant. Another example concerns the theoretical and computational molecular science group. In the last few years, this group has been very strong indeed under Prof. Ishizaki (an expert in condensed phase quantum dynamics), Prof. Ehara (an expert in electronic structure theory), and Prof. Saito (an expert in statistical mechanics and simulation). However, Prof. Ishizaki has recently accepted an offer from Toyko University, and Profs. Ehara and Saito are both approaching retirement age. The search for a replacement for Prof. Ishizaki is already underway, and I hope the planned increase in retirement age for those with active research grants will help the IMS to retain Profs. Ehara and Saito for a while longer before they too are eventually replaced.

### 4. Final thoughts and a recommendation

The "no promotion" policy of the IMS is a contentious one that has been highlighted in several previous reports on the institute. Historically, the policy seems to have succeeded in its goal. The vast majority (more than 80%) of previous IMS Associate Professors have in fact been promoted to positions elsewhere, and more than 90% of these have moved to Full Professorships at universities in Japan. Since the brightest researchers are often the best teachers, and there is no undergraduate teaching at IMS, this has clearly been beneficial for the education of Japanese scientists. However, the policy is problematic for the few who do not manage to secure outside promotions, and potentially also for the institute itself, since these people are then stuck in IMS with no foreseeable career development until retirement. Encouraging these people to apply for promotions at provincial universities and/or alternative roles within IMS (such as university research administrators) is clearly sensible. But more importantly, my impression from some of the conversations I have had during this visit is that the recruitment and retention of Full Professors at IMS is becoming more difficult than it once used to be. Given this, and the fact that the institute nurtures some of the very best Associate Professors in Japan, it does seem strange to me that they are not allowed to apply for Full Professorships at IMS when they become available, in competition with external candidates. This would not significantly impact the flow of scientific talent from IMS to the universities, since the competition with external candidates would ensure that internal promotions remained rare. But it would give the IMS more scope to hire the best possible candidates to its Full Professorships and thereby help to safeguard its future international standing.

# 5-3　物質分子科学研究領域の評価

## 5-3-1　Mischa Bonn 外国人運営顧問

**Assessment of the Institute for Molecular Science, Okazaki**

**By Mischa Bonn, Max Planck Institute for Polymer Research, Mainz, Germany**

### Overall Impression of IMS

The Institute for Molecular Science (IMS) is a center of research excellence tackling important challenges in molecular sciences. It has outstanding research outputs and has launched the careers of many successful scientists who have gone on to professorships at other institutions. The Institute's strengths include highly motivated staff performing at the highest level, outstanding leadership, and equipment/instrumentation that exceeds that of many world-class laboratories internationally. The research facilities are well-organized and well-maintained by dedicated technical and research staff, and they are open to the public and local research groups. As such, the scientific infrastructure benefits both the local scientific endeavors and molecular science throughout Japan. IMS hosts numerous outstanding scientific groups covering a broad range of fields, with a tangible mission to foster interdisciplinary research at the intersection of physics, chemistry, and materials science. The Institute maintains a high level of scientific and technological excellence, making it one of Japan's most internationally visible research centers. The UVSOR Synchrotron Facility is well-suited to an institute of IMS's size and provides unique capabilities for experiments in material science and biological applications. The integration of this user facility into the diverse scientific environment at IMS provides important added value. IMS plays a crucial role in the Japanese scientific landscape, by providing both research facilities and opportunities for researchers to become fully independent at a much earlier stage than is traditional in Japanese universities.

The Institute for Molecular Science (IMS) has demonstrated a bold and visionary approach to recruitment, consistently providing exceptional young scientists with the necessary resources and support to flourish in their research endeavors. This strategic investment in emerging talent has yielded remarkable results, with nearly 100 staff members advancing to prestigious positions such as professorships at other esteemed institutions over the course of its 49-year history. The IMS stands as a beacon of excellence in the Japanese scientific community, serving as a fertile ground for nurturing and developing the next generation of scientific leaders. Its commitment to fostering innovation and cultivating talent has solidified its position as a crucial incubator for cutting-edge research and a cornerstone in shaping the future of molecular science both within Japan and on the global stage.

Opportunities for improvement and strategic recommendations:

1. **Group Size:** IMS research groups tend to be smaller than international competitors, limiting their ability to quickly capitalize on breakthroughs. Contributing factors may include personnel budget constraints and challenges in recruiting top students due to limited integration with universities (see also points 2 and 3).

2. **Enhance Financial Resources for Global Competitiveness:** To maintain its position as a world-class research institution, IMS must prioritize securing additional funding. While the Institute's budget has remained stable relative to Japan's GNP over the past three decades, the lack of economic growth has resulted in a static financial situation. This presents challenges in an increasingly global, highly competitive research landscape. Additional funding is essential for:
    - Equipment Modernization: Allocate resources to replace aging infrastructure with state-of-the-art technology.

- Expansion of Research Teams: Increase funding to support larger, more robust research groups capable of tackling complex scientific challenges.
- International Talent Acquisition: Secure funds to attract and retain top-tier researchers from around the world.
- Retaining a Competitive Edge: Ensure IMS remains at the forefront of molecular science by investing in cutting-edge projects and collaborations. Continue to leverage and expand on the strengths of facilities like UVSOR and the interdisciplinary nature of IMS to maintain its position as a world-leading research institute.

By actively pursuing increased funding through various channels, IMS can reinforce its critical mass of resources and talent. This financial boost is essential for the Institute to keep pace with and lead the international scientific community.

3. **University Integration / PhD Student Recruitment:** Consider developing stronger relationships with universities to improve access to potential PhD students and young researchers. A concrete suggestion would be to initiate an active alumni network (for instance, on the occasion of the 50$^{th}$ birthday of the IMS) and/or initiate an exchange student program where students (from these alumni) can come to IMS for extended stays of defined length (*e.g.*, six months, one year, or two years). The competition for PhD students among Japanese universities and research institutes like the Institute for Molecular Science (IMS) is expected to intensify in the coming years due to the projected decline in the student population. This demographic shift necessitates the urgent development of a comprehensive strategy to attract high-quality students, both domestically and internationally. The IMS could consider developing cross-disciplinary programs in emerging scientific frontiers that resonate with a wider spectrum of students. Simultaneously, simplifying application procedures and offering comprehensive support services for international students can remove barriers to entry and enhance the institution's global appeal. Additionally, effectively utilizing digital platforms and social media to highlight research accomplishments and share student experiences can significantly boost visibility and engagement with potential candidates worldwide.
4. **Promotion Policy:** The non-promotion policy for Assistant or Associate Professors within IMS may be a barrier for some researchers, particularly those looking to establish stable roots for family reasons. While I appreciate the reluctance to install a tenure-track model for Assistant or Associate Professors, IMS scientists should be allowed to apply for openings at the Institute. This should be unproblematic given the clear and transparent procedures for appointing new staff.
5. **Gender Balance:** There is a significant underrepresentation of women at the Principal Investigator (PI) level. While this gender disparity is a widespread issue across Japan, the IMS, given its influential position in the country's scientific community, has a responsibility to take proactive steps to address and improve this imbalance. As a leading institution, IMS can set an example by implementing measures to increase female representation in senior research roles, thereby contributing to broader efforts to enhance gender diversity in Japanese academia. Address gender imbalance by actively seeking input from female professors and PhD students on barriers and potential solutions. Implement policies that specifically support women in science, such as providing additional research support during family leave.

In the following, I will provide my observations on the IMS researchers and facilities in the sequence they were introduced to me. My commentary will begin with the individuals and facilities I was explicitly requested to evaluate more thoroughly, followed by those for which I was asked to offer brief remarks.

Assessment of individual researchers

**Prof. Hiroshi Yamamoto**

Prof. Hiroshi Yamamoto's outstanding research focuses on organic electronics and spintronics, aiming to revolutionize future electronic devices through the development of organic superconductors and molecular spintronics. His excellent work is centered on novel mechanisms such as electric-field-induced superconductivity in organic field-effect transistors (FETs) and chiral molecular systems to explore the mechanism behind the chirality-induced spin selectivity (CISS) effect. He cleverly bridges the fields of organic and inorganic superconductors. His contributions aim to enhance device mobility and efficiency in the next generation of electronic materials through a fundamental understanding of the physics involved.

Key Strengths:

- Innovative Device Development: Prof. Yamamoto has pioneered organic chiral superconductors to study the CISS effect, setting new standards in such studies.
- Cross-Disciplinary Impact: His research merges organic chemistry, physics, and material science, impacting not only electronics but also superconductivity and spintronics.
- Recognized Excellence: His work is well-cited and has garnered accolades, affirming his leadership in material sciences.

**Assoc. Prof. Katsuyuki Nishimura**

Associate Professor Katsuyuki Nishimura's research is focused on solid-state NMR spectroscopy of biological and material-science systems. His research aims to develop novel solid-state NMR techniques for studying membrane proteins and misfolded protein assemblies, *i.e.*, amyloids. The goal is to elucidate structure–function relationships in these systems. Dr. Nishimura has established productive collaborations combining NMR with other biophysical methods. His work contributes significantly to our understanding of membrane protein structure and dynamics.

Key strengths:

- Development of novel solid-state NMR techniques, including exceptionally high-rate MAS devices, for studying membrane proteins and complex molecular materials
- Elucidation of structure–function relationships in important membrane proteins
- Productive collaborations combining NMR with other biophysical methods

**Prof. Toshihiko Yokoyama**

Prof. Toshihiko Yokoyama specializes in surface and interface science, particularly investigating the structural and electronic properties of surfaces and nanomaterials. His research on surface phenomena such as adsorption, catalysis, and thin-film growth contributes to advancements in nanotechnology and energy materials. His *operando* hard x-ray photoelectron spectroscopy (HAXPES) is particularly admirable, having been applied to various complex, important systems, including heterogeneous catalysis, electrochemistry, and Nafion membranes. The ability to probe the local electrochemical potentials and oxidation states is very impressive. In an independent line of research, the atomic origin of the zero thermal expansion of specific alloys is investigated.

Key Strengths:

- Pioneering Surface Science: Prof. Yokoyama's work substantially advances our understanding of active material interfaces, which is crucial for technology applications.

- Leader in Energy Materials: He is at the forefront of exploring the electronic properties of surfaces at the nanoscale, with the perspective of enhancing material performance in various technologies.
- Enables advanced photoelectron spectroscopy for a large community with the *operando* HAXPES setup, which is now available as a user facility at a beamline.

**Senior Researcher Taketoshi Minato**

Taketoshi Minato's excellent research program focuses on energy conversion processes at molecular interfaces, particularly in relation to electrode/electrolyte interfaces. Despite being a relatively recent addition to the faculty, Taketoshi Minato has an impressive track record in both developing new measurement techniques, using *operando* surface probe microscopy (SPM), and applying these tools to critical challenges in energy conversion systems. The ability to extract both the elastic modulus and adhesive force from the SPM force curve provides detailed insights into the electrode–electrolyte interface. This approach allows Minato to quantitatively assess mechanical properties and adhesion characteristics at the nanoscale, elucidating complex physicochemical processes and enhancing our understanding of interfacial phenomena. In a second line of work, mechanistic insights into a new type of battery, the fluoride shuttle battery, are obtained. His work involves understanding how these molecular interactions at surfaces can be harnessed to improve energy efficiency and create more sustainable technologies.

Key Strengths:

- Interfacial Chemistry Expertise: Minato excels in unveiling energy conversion at molecular interfaces, improving catalysis processes.
- Focus on Sustainability: His research addresses critical challenges in renewable energy, particularly in battery technologies.
- Technological Application: Minato's work can translate into practical improvements in energy technologies, bridging fundamental science with real-world applications.

**Prof. Toshikazu Nakamura**

Prof. Nakamura is a prominent researcher at the Institute for Molecular Science (IMS), contributing significantly to the field of spin-based molecular systems. His research is centered on low-dimensional, highly correlated electron systems and functional materials, with a focus on understanding electron spin dynamics and the functionalities of these systems at low temperatures. His investigations primarily involve molecular-based conductors, employing advanced techniques such as broad-line NMR (Nuclear Magnetic Resonance) and ESR (Electron Spin Resonance) to study electronic phases and the role of spin in complex molecular environments. One of the central goals of Nakamura's work is to explore how competition between electronic phases in these systems can lead to novel functionalities. His studies have implications for developing materials with unique electronic properties, which could play a role in next-generation technologies, including quantum computing and spintronics. A notable project under his leadership is the MEXT CURE Program, "Frontiers of Spin Life Sciences, Spin-L," which aims to bridge the gap between life sciences and spintronics by understanding the role of electron spins in biological and molecular systems. This interdisciplinary approach seeks to uncover novel applications of spin in fields such as biomedicine and material science, reflecting Nakamura's commitment to pioneering new frontiers in science.

Key Strengths:

- Interdisciplinary Vision: Prof. Nakamura is a leader in pushing the boundaries between molecular science and spintronics, as seen in his involvement in the Spin-L program. His research not only advances fundamental physics but also applies this knowledge to life sciences, an innovative approach that opens up new avenues for scientific exploration.

- Expertise in Advanced Measurement Techniques: His proficiency in techniques like ESR allows him to delve deeply into the quantum behaviors of electron systems, providing precise insights into spin dynamics, and photo-injected charge carriers. These advanced techniques are crucial for investigating complex materials that are not well understood through conventional methods.
- Pioneering in Functional Material Discovery: Prof. Nakamura's research contributes to the discovery of new materials with potential applications in fields like quantum computing and spin-based electronics.

**Prof. Shin-ichi Kimura**

Prof. Shin-ichi Kimura is a distinguished researcher in solid-state physics and spectroscopy, holding joint appointments at Osaka University's Graduate School of Frontier Biosciences and the Institute for Molecular Science (IMS). This unique dual position allows him to leverage the strengths of both institutions, fostering interdisciplinary research and collaboration. His research focuses on elucidating the electronic states of materials and their interactions, fundamental to understanding physical properties and life phenomena. Prof. Kimura's research approach is distinctive in its dual focus. He excels in both the development of advanced beamline instrumentation and the application of these cutting-edge tools to investigate compelling scientific questions, particularly in the field of correlated electron systems. This synergistic combination of technical innovation and fundamental research allows him to push the boundaries of experimental capabilities while simultaneously addressing critical problems in condensed matter physics. This work aligns well with both institutions' goals, advancing our understanding of molecular systems from different perspectives. The joint appointment allows Prof. Kimura to access diverse resources and expertise, enhancing his research capabilities. Simultaneously, both institutions benefit from his broad knowledge and experience, fostering a dynamic research environment that spans traditional disciplinary boundaries. I understand that Prof. Kimura's appointment at IMS is up for renewal shortly. I strongly support that renewal.
Key strengths:

- Expertise in Advanced Spectroscopic Techniques: He has developed novel methods using synchrotron radiation and quantum beams to visualize changes in electronic states, benefiting both institutions with cutting-edge research tools.
- Interdisciplinary Research Approach: His work bridges physics, chemistry, and life sciences, investigating topics from solid-state physics to biological molecules. This broad perspective enriches both Osaka University's biosciences program and IMS's molecular science focus.
- Collaborative Network Builder: Prof. Kimura's dual role facilitates strong connections between Osaka University and IMS, promoting joint research projects and knowledge and student exchange.

**Assoc. Prof. Toshiki Sugimoto**

Assoc. Prof. Toshiki Sugimoto's excellent research program focuses on developing new, highly sensitive techniques, and applying those techniques to complex (photocatalytic) systems. Sugimoto and his team developed a novel approach using *operando* FT-IR spectroscopy under varying humidity, synchronized with periodic excitations of photocatalysts. This has allowed them to directly quantify the water-film-thickness-dependent photocatalytic hydrogen evolution on metal-loaded oxides.
These contributions demonstrate Sugimoto's ability to develop novel experimental techniques and apply them to gain deep insights

into complex photocatalytic systems, advancing our understanding of surface chemistry and catalysis.

Key Strengths:

- Deep Insights into Complex Photocatalytic Systems: Sugimoto's work has provided microscopic insights that shift the paradigm on the role of water in photocatalysis. This understanding offers a fundamental basis for the rational design of metal/oxide complex interfaces for efficient hydrogen evolution and methane upcycling.
- Technical Innovation: Sugimoto has developed STM-based near-field surface-specific SFG spectroscopy, a cutting-edge technique allowing unprecedented spatial resolution in studying molecular systems at surfaces. This innovation combines the high spatial resolution of scanning tunneling microscopy (STM) with the chemical specificity of sum-frequency generation (SFG) spectroscopy, enabling detailed investigations of surface reactions and dynamics at the molecular level.

**Prof. Hiroshi Onishi**

Prof. Hiroshi Onishi holds a cross-appointment position as a Professor at both Kobe University and the Institute for Molecular Science (IMS). His research focuses on surface science, catalysis, and energy-related chemistry, with particular expertise in scanning probe microscopy and optical spectroscopy. Prof. Onishi is a nationally and internationally highly visible ambassador for IMS. Key strengths of Prof. Onishi include:

- Pioneering Work in Atomic Force Microscopy (AFM): He has made significant contributions to the development and application of AFM techniques for studying surfaces at the atomic level.
- Expertise in Surface Chemistry: His research provides deep insights into chemical reactions occurring at solid surfaces, particularly in catalytic processes.
- Interdisciplinary Approach: Onishi combines advanced microscopy techniques with spectroscopy to elucidate complex surface phenomena.

Recently, Prof. Onishi has made notable achievements in performing high-level AFM studies of ice surfaces. His work has revealed unprecedented details about the structure and behavior of ice at the molecular level, contributing to our understanding of ice physics and chemistry. These studies have implications for various fields, including atmospheric science and materials engineering. The cross-appointment between Kobe University and IMS brings significant added value to both institutions. At IMS, Prof. Onishi brings his knowledge and experience to cutting-edge facilities and a collaborative environment with experts in molecular science. This arrangement allows him to combine the strengths of both institutions, fostering interdisciplinary research and enabling more comprehensive studies of surface phenomena. The synergy between the two institutions enhances the impact and scope of the research, particularly in the areas of surface science and catalysis. I, therefore, recommend extending the cross-appointment until Prof. Onishi's retirement at Kobe in March 2028.

Comments on specific facilities

**IMS Instrument Center**

The Instrument Center at the Institute for Molecular Science (IMS) is a pivotal facility providing advanced equipment and technical support for molecular research. It houses cutting-edge instruments like high-resolution electron microscopes, NMR spectrometers, mass spectrometers, and synchrotron radiation tools. These resources enable researchers to conduct high-precision experiments in fields such as molecular spectroscopy, surface science, and material chemistry.

The center fosters collaboration between IMS researchers and external institutions by providing access to its sophisticated facilities. This collaborative approach supports cross-disciplinary studies, contributing to advancements in molecular sciences. Additionally, the center emphasizes continuous innovation, upgrading its instruments and developing new methodologies to stay at the forefront of research.

Another core strength of the Instrument Center is its commitment to education and training. The center's expert staff provide hands-on training for young researchers, offering guidance in the use of complex equipment and data interpretation. This ensures efficient experimentation and supports the professional development of students and early-career scientists.

Key strengths of the Instrument Center:

- State-of-the-Art Equipment: Cutting-edge instruments for high-precision molecular research.
- Collaborative Support: It promotes inter-institutional collaboration, driving innovation.
- Comprehensive Training: Offers essential guidance and training, contributing to skill development in molecular sciences.

In sum, the IMS Instrument Center is essential for advancing molecular science, fostering innovation, and developing future scientific leaders.

### Comments on other IMS researchers and infrastructure

**Prof. Shuji Akiyama** is a distinguished researcher, specializing in biophysics and chronobiology. His work focuses on elucidating the molecular mechanisms of circadian clocks, particularly in cyanobacteria. Akiyama has made significant contributions to understanding the KaiABC oscillator system, employing advanced techniques such as X-ray crystallography and NMR spectroscopy. His research has provided crucial insights into the structural basis of circadian rhythms and protein–protein interactions in clock systems. Akiyama's innovative approaches have led to breakthroughs in visualizing the dynamic processes of circadian oscillations at the molecular level. As a professor in the Department of Life and Coordination-Complex Molecular Science, Akiyama continues to push the boundaries of chronobiology research, combining structural biology with biophysical techniques to unravel the complexities of biological timekeeping mechanisms.

**Prof. Yasuhiro Uozumi** is a renowned professor, specializing in organic synthesis and catalysis. His recent work on photocatalytic conversion has garnered significant attention, particularly for its innovative approaches to sustainable chemistry. Uozumi's research focuses on developing novel photocatalysts that demonstrate enhanced activity and selectivity in various organic transformations. By utilizing visible light for these reactions, he has made strides in reducing the need for harsh reagents and conditions, aligning his work with the principles of green chemistry. Notably, he has pioneered the use of water as a reaction medium for photocatalytic conversions, further promoting environmentally friendly practices. The implications of Uozumi's research extend beyond academia, with potential applications in pharmaceutical synthesis and fine chemical production. His impressive contributions to photocatalysis not only address critical challenges in modern chemistry but also pave the way for more efficient and sustainable production processes across various industries.

**Assoc. Prof. Hikaru Kuramochi** is a highly accomplished ultrafast molecular spectroscopist at the Institute for Molecular Science. His work focuses on elucidating the function, structure, and dynamics of condensed-phase molecular systems using advanced ultrafast laser spectroscopy. He develops new techniques and applies these to important questions in the field. His expertise in ultrafast and nonlinear spectroscopy has led to notable publications, including studies on protein dynamics and photoisomerization. Kuramochi's innovative research extends to developing highly sensitive and ultrafast electronic spectroscopy for visualizing multi-dimensional chemical reaction dynamics. His ongoing projects and collaborations continue to push the boundaries of molecular science, making him a valuable asset to the Institute for Molecular Science.

**Prof. Kenji Ohmori** is a world-renowned physicist and chemist, with a remarkable track record. Ohmori's outstanding research program focuses on 'fast and cold': Ultrafast spectroscopy, coherent control, and quantum information processing using cold atoms. His notable achievements include developing ultrahigh-precision coherent control techniques and pioneering work on visualizing quantum wave packet interference. Prof. Ohmori's contributions to molecular science and quantum computing are recognized world-wide and his work has accordingly been published in high-impact journals. His research continues to push the boundaries of quantum control and molecular dynamics, with major potential applications in quantum computing.

**Prof. Hiromi Okamoto** leads groundbreaking, internationally well-connected research on nanomaterial optical properties. His work primarily involves developing and using near-field optical microscopy to investigate chiral light–matter interactions. His group has made significant advances in visualizing wave functions of nanostructures and exploring local optical activity, which includes the observation of strong localized optical fields in gold nanoparticles, as well as local chiral fields around achiral structures. Recent achievements include demonstrating high selectivity for left- or right-handed circularly polarized light using chiral gold nanoparticles. The prospect of making these technologies available to the wider scientific community by commercializing the CD microscope is very appealing. The outlook of inducing chirality in molecular systems to create chiral (supramolecular) structures is very exciting and innovative. These advancements highlight his contributions to nanophotonics and plasmonics, pushing the boundaries of how we visualize and manipulate light at the nanoscale.
Given that a recently appointed assistant professor is currently on maternity leave, coupled with the demonstrated excellence and promising nature of the research being conducted, I recommend extending the group's tenure by 1–2 years. This extension would provide the necessary time to compensate for the temporary absence, ensure continuity in ongoing projects, and allow the group to realize exciting research plans. It would also demonstrate support for work-life balance and recognize the value of the research contributions made thus far.

**Prof. Shinji Saito** specializes in theoretical and computational studies of molecular dynamics. His research delves into the complex behaviors of many-body molecular systems, such as liquids and biomolecules, with a focus on energy dynamics in light-harvesting complexes, aqueous and other liquid systems, and glass transitions. He explores dynamic heterogeneity, a critical concept for understanding the glass transition and reactions in fluctuating environments. His work connects to multidimensional spectroscopy through multi-time correlation functions to study these dynamic processes at both the collective and single-molecule levels, revealing how biomolecular conformational changes influence their functions. Key strengths of Prof. Saito include his deep theoretical insights into molecular behavior, particularly in explaining the non-uniform dynamics in supercooled liquids and biomolecular systems. He is also renowned for his innovative application of advanced computational techniques, such as higher-order nonlinear spectroscopy, to elucidate reaction and conformational dynamics. Finally, his interdisciplinary approach, linking theoretical chemistry with experimental insights, has provided a comprehensive understanding of both biological and physical systems at the molecular level.

His contributions have significantly advanced our understanding of molecular dynamics, particularly in systems with complex environments.

**Prof. Fumihiko Matsui** leads pioneering work at the UVSOR Synchrotron Facility. His research focuses on advanced photoemission methodologies, particularly through the use of the photoelectron momentum microscope (PMM). His team aims to investigate the behavior of electrons and electron spins in novel spin materials, which is crucial for understanding magnetism, superconductivity, and topological properties. One of Dr. Matsui's major contributions is the construction and development of the PMM at UVSOR, enabling 3D spin vector imaging and resonant photoelectron diffraction spectroscopy. His work has revolutionized the analysis of electronic structures and valence band dispersions with high spatial resolution. These efforts are critical for advancing the understanding of complex materials and their applications in various technological fields.

**Prof. Masahiro Ehara** is a leading researcher focusing on advancing computational chemistry to understand complex chemical systems, in addition to being head of the Research Center for Computational Science. His scientific work significantly contributes to quantum chemistry and photochemistry, where he develops state-of-the-art electronic structure theories to examine light-matter interactions. Notably, Ehara's research on time-dependent light-matter interactions involves using advanced theoretical models to also calculate the effects of solvent and excited states. These approaches have applications in understanding the behavior of molecules under light excitation and in catalysis. His group successfully explores a remarkably wide range of topics, including photophysical chemistry, heterogeneous catalysis, and metal nanoclusters, applying quantum chemical calculations to develop efficient catalytic systems. His work helps bridge the gap between theoretical chemistry and real-world applications in fields like energy and materials science.

**Assoc. Prof. Takashi Kumagai** is a leading researcher in the field of nanoscale molecular science. His outstanding work focuses on advancing scanning probe microscopy techniques to observe and manipulate single molecules with unprecedented precision. Kumagai has made seminal contributions to single-molecule chemistry, directly observing reactions like tautomerization in porphycene molecules. His research has also demonstrated the ability to visualize quantum dynamics at the atomic level, such as hydrogen transfer via quantum tunneling. Recently, Kumagai's team achieved a major breakthrough by successfully observing vibrational spectra of single proteins using near-field infrared nanospectroscopy. This technique allows for detailed analysis of extremely small samples, overcoming the limitations of conventional infrared spectroscopy. Kumagai's innovative approach combines scanning probe microscopy with plasmonics to develop novel nanoscale spectroscopy methods with exceptional spatial and temporal resolution.

### Brief comments on facilities

**The Research Center for Computational Science (RCCS)** plays a vital role in supporting computational research across molecular science and bioscience. Its mission is to provide large-scale computation services that surpass the capacities available at typical university computer centers, making it a crucial resource for complex simulations in molecular and material science. The RCCS supports researchers by offering advanced hardware and software environments, program libraries, and databases, ensuring that scientists can execute high-performance, large-scale calculations with ease. For the next generation of computational researchers, the Center provides schooling on different aspects of computational Chemistry and Physics. One of the very impressive statistics is the large number of yearly publications (~600) enabled by contributions from RCCS, relative to the number of unique users (~1000) and groups (~300, numbers from 2020). The number of users has been rapidly increasing in the past few years. With state-of-the-art computational resources and dedicated support staff, the RCCS remains at the forefront of computational research, driving innovations that benefit a broad spectrum of scientific fields.

**The UVSOR Synchrotron Facility** is a unique, highly specialized synchrotron radiation facility, with a focus on generating extreme ultraviolet light and soft X-rays for cutting-edge research in multiple fields. Following its upgrade to the UVSOR-III model in 2012, the facility now boasts one of the highest brilliance levels for sub-1 GeV synchrotron light sources. The facility operates 14 beamlines, including “Open beamlines” accessible to a broad range of researchers and “In-house beamlines” used exclusively by IMS teams. These beamlines enable advanced studies in molecular science, materials physics, life sciences, and solid-state physics. Key research achievements include photoelectron spectroscopy, the development of gamma-ray sources, and the exploration of new light sources for nanomaterials and biological systems. The UVSOR facility supports various academic and industrial applications, including nanotechnology and biomedicine, and is actively engaged in developing next-generation microscopy and spectroscopy techniques.