7-2　外国人運営顧問による点検評価

7-2-1　Benjamin List 外国人運営顧問

Dear Professor Kawai,

Thank you very much for giving me the opportunity to serve on the Scientific Advisory Board of the Institute for Molecular Science, of which you are the Director General, and which belongs to the National Institutes of Natural Sciences. It has been an honor to meet you and to have an on site visit from November 13th to November 14th at your institute. You have kindly presented to me the history, funding, structure, and science conducted at your impressive institute. I have also had the pleasure to be personally introduced to your individual departments by their department heads, including the Department of Materials Molecular Science, headed by Professor Toshihiko Yokoyama, the Department of Theoretical and Computational Molecular Science, headed by Professor Shinji Saito, the Department of Life and Coordination-Complex Molecular Science, headed by Professor Yasuhiro Uozumi, and the Department of Photo-Molecular Science, headed by Professor Kenji Ohmori. Furthermore, I have been given the opportunity to visit the IMS research facilities, including the UVSOR Facility, and the Research Center for Computational Science. Finally, as part of my duties, I had the pleasure to hold individual interviews with the members of the Department of Life and Coordination-Complex Molecular Science (Professor Koichi Kato, Assoc. Professor Norie Momiyama, Assoc. Professor Shigeyuki Masaoka, Professor Ryota lino, Professor Shigetoshi Aono, Professor Yasuhiro Uozumi, Assoc. Professor Yuji Furutani, and Res. Assoc. Professor Kensuke Kurihara).

My overall impression of both, the institute in general and the Department of Life and Coordination-Complex Molecular Science in particular, has been excellent.

Before discussing specific aspects of the Department of Life and Coordination-Complex Molecular Science, I would like to take this opportunity, to make a few general remarks concerning your institute.

First of all, I noticed that there are several similarities to my own institution, the Max-Planck lnstitut für Kohlenforschung, and to the Max-Planck-Society in general. But there are also differences. For example, both of our institutes have five departments. While our institute has about 350 employees, including scientist as well as administrative and service members, and has a budget of around €27 million, the IMS has fewer employees (277) but a slightly higher budget (4 Billion Yen, ca. €29 million). Accordingly, one coworker on average costs around €105,000 per year at the IMS, whereas at my institute, on average, one person costs €77,000 per year. I am not sure, how to explain this difference. Perhaps income and cost of living are generally higher in Japan. I was also considering the possibility that the large infrastructural costs of your synchrotron beam line is responsible for this difference. However, from what I learned, it costs only 6% of your annual budget.

A significant difference can be seen both in the number of groups in each department and also in the individual group sizes. While your departments on average have eight groups, at our institute there are merely three. I would assume that spreading your resources among so many groups is expected to increase the chances of a scientific “hit.” On the other hand, some of your groups are clearly subcritical and even non-competitive regarding manpower. In the Max Planck Society we have a different philosophy and give each department's director the complete freedom as to how he or she uses the resources allocated to the department. This typically leads to much larger groups of the director, which can be a quite powerful scenario. Sometimes, a diminished scientific diversity may result in such departments, but overall such a funding situation is possibly more attractive for the top scientists we aim to recruit. Possibly, reducing the number of groups in each department or giving each director the freedom to decide how many groups he deems suitable for his department is something for you to consider. This may also be discussed at the National Institutes of Natural Sciences.

Another aspect concerns the quest for recruiting outstanding scientists. In my opinion, to meet these challenges, a very high level of flexibility is required. In the Max Planck Society, we have similar rules like you, according to which assistant professor or associate professor level scientists cannot be promoted to director, which is our full professor level. However, we keep the flexibility to promote junior level group leaders, in very few exceptional cases (probably less than 1%), to the position of a director. Why would we voluntarily ask our most outstanding scientists to leave the society? My advice would be to seriously consider this model also for the IMS. I have seen amazing younger talents at your institute, some of which clearly have the caliber for top positions, be it at the MPG or at your institute or anywhere else in the world.

A minor recommendation concerns the names of your departments. I personally favor short names. For example, you may consider "Theory," "Light," "Materials," and "Life and Synthesis." Obviously, this is a matter of taste and I realize that this may well not meet yours or that of Japanese scientists in general. Also, a clear mission of the institute that can be expressed in one sentence may be helpful.

With regards to the group leaders of the Department of Life and Coordination-Complex Molecular Science, I would like to say the following: The order of individual group leaders follows the order of my interaction with them. (First Day: 1. Koichi Kato, 2. Norie Momiyama, 3. Shigeyuki Masaoka, 4. Ryota lino, 5. Shigetoshi Aono. Second day: 6. Yasuhiro Uozumi, 7. Yuji Furutani, 8. Kensuke Kurihara)

1. **Professor Koichi Kato**: Professor Kato heads the Division of Biomolecular Function. In a nutshell, the highly ambitious aims of this group are to understand how life self-assembles from molecules, and ultimately to create life. I would say that this group works on one of the grand challenges of not only chemistry and biology but also of mankind. This question is perhaps paralleled by the quest of physicists to find the Grand Unified Theory, or to understand dark matter. Obviously, such a big problem cannot be solved by one group only and requires the collaborative effort of diverse scientists. These include synthetic chemists as well as experts from spectroscopy (NMR, IR, *etc.*), cryo-EM, Mass Spectrometry, and computation. It is highly impressive how Professor Kato oversees all these activities and how he collaborates with various scientists all over the planet that are engaged in the few missing areas that he is not covering himself. He has a keen and authentic interest in a real "synthetic biology" and also has been highly successful in establishing major consortia towards such a science. Examples of his particular activities include the investigation of how protein glycosidation patterns govern their biological fate and also how the proteosome assembles, which is probably one the most complex supramolecular events in life. His interdisciplinarity, ambition, and scientific excellency is internationally well-recognized. His research is outstanding and I am confident that this world class group is among those at the institute that have the potential to publish

major papers in the very top journals such as *Nature* and *Science*.

2. **Assoc. Professor Norie Momiyama**: I can probably judge her work best, since my research interests overlap significantly with hers. She studies asymmetric organocatalysis and has, in a relatively short time at the institute, already made significant, original, and highly noticeable contributions. Specifically, she is engaged in three complementary projects: 1. she has discovered a fascinating and rather unexpected rearrangement reaction of butenyl amines with aldehydes. The mechanism of this reaction is being elucidated very carefully in her lab and in collaboration with Professor Suzuki, also at the IMS. This group also designs and develops new catalysts for asymmetric Brønsted acid catalysis. Finally, the Momiyama group develops new concepts within the area of halogen bonding. For example, they discovered a halogen bonding mediated allylation of heteroaromatics. Even more impressively, they immobilize organocatalysts onto polymers that possess halogen bonding sites. The resulting heterogeneous catalysts are very active and can be used in a synthesis of amino acids. Taken together, Professor Momiyama is clearly a very good scientist and leads a group that does promising and highly original research in the area of organocatalysis. She has a very keen interest in mechanistic questions and has clearly the potential to become an excellent professor in the near future.

3. **Assoc. Professor Shigeyuki Masaoka**: This group is engaged in extremely relevant problems such as the water oxidation, the CO_2 to CO reduction, and the N_2 to NH_3 conversion. All of these processes have the potential to make a massive impact for human life on earth. The group has recently had a major breakthrough with the discovery of a well-designed water oxidation catalyst based on a pentanuclear iron cluster (*Nature* **2016**, *530*, 465). By solving the overpotential problem, their spectacular system catalyzes the water oxidation with rates higher than its natural counterpart. In addition, they are extremely meticulous in elucidating the mechanism of their reaction. In fact, each intermediate has been carefully characterized by cyclic voltammetry, DFT studies, Mössbauer spectroscopy, and the synthesis of individual intermediate states. They also have made impressive progress in the other areas of their interest, including fuel production from CO_2, photo-induced electron transfer, and active site assembly. Congratulations to Professor Masaoka for these amazing results and to the institute for hiring such an outstanding scientist.

4. **Professor Ryota Iino**: Professor Iino is interested in molecular machines. It is rather fascinating to note that while in biology essentially all of the key systems, including ATPase and many others, involve spectacular molecular motors, chemists are still far away from being able to produce even simplistic synthetic analogs. This is where the group makes its impact. Professor Iino and his team want to build molecular motors using computational design and directed evolution but they also intend to build hybrid or chimera that combine synthetic structures with biological entities. Towards these goals, in addition to computational work and saturation mutagenesis studies, they use a plethora of techniques such as optical MS, AS-AFM, x-ray and neutron diffraction, CryoEM. They also intensely collaborate with many other groups both at the IMS (with physicists at the photo department and with theory department) but also with other institutions in Japan and around the globe. They have published their excellent results in high ranking journals, including in the *Proceedings of the National Academy of Sciences (PNAS)*, in *Angewandte Chemie* and in *Nature Chemical Biology*.

5. **Professor Shigetoshi Aono**: Professor Aono's research interests are in the general area of bioinorganic chemistry. For his research he relies on protein crystallography and on biochemical methods. Key findings of this very good group include the study of sophisticated

iron uptake mechanisms that bacteria have developed, which rely on the chemical recycling of heme molecules of their hosts. His group also studies how heme regulates gene-expression and how vitamin B12 can function as an unexpected photosensing unit.

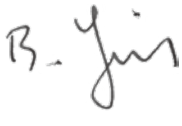
6. **Professor Yasuhiro Uozumi**: Professor Uozumi is a world-wide leader in the area of catalysis design and engineering. He continues to be an inspiration to many in advancing spectacular catalyst systems with properties that approach perfection. For example, they have developed hyperactive catalysts with ppb level activity. The group has also pioneered flow chemistry. The main inspiration of Professor Uozumi comes from enzyme catalysis but not in the sense that they try to make synthetic analogs but more in terms of learning from the key reactivity driving forces, which include a hydrophobic pocket, water-based conditions, and the utilization of transition metal complexes. On the basis of these considerations, they have developed amphiphilic resins that have led to extremely active and recyclable catalysts for applications in water. Examples include sub-ppm catalysis of the Suzuki reaction, and Heck reaction catalysts that approach one billion turnovers! He has also developed fascinating polymeric Brønsted acid catalysts that can be used to make biofuel. A particularly interesting topic is the immobilization of Pd-catalysts onto silicon wafers. The resulting catalysts can be recycled >100 times. The group publishes their excellent results in many papers in different journals.

7. **Assoc. Professor Yuji Furutani**: Since many years, Professor Furutani is interested in using infrared spectroscopy to study protein function. Considering that he has a very small group (two additional members), his group has made very good progress, even though he works in an extremely competitive research field. They collaborate with the group of Professor T. Fuji at the photo department of the IMS. The group is specifically interested in studying potassium channels and they have published very well in this area. FTIR is established by Professor Furutani and his team as an ideal tool to investigate membrane proteins, which are notoriously difficult to study using crystallography. This is where the group can make a strong impact in the future.

8. **Research Assoc. Professor Kensuke Kurihara**: This team aims at the formidable challenge of creating artificial cells. They use the more difficult bottom-up approach in contrast to the top down approach used by other groups around the world. They have elegantly studied oil droplet protocells that self-reproduce. They also study interesting approaches of using in situ generated amphiphilic catalysts from an oily amine and an aldehyde catalyst. It will be interesting to follow the development of this laboratory in the future.

Thank you very much again for giving me the opportunity to visit and learn about IMS. It has been both a pleasure and an inspiration to serve your excellent institute.

Best regards,



Professor Benjamin List,
Professor of Chemistry at the University of Cologne and Director at the Max-Planck-lnstitut für Kohlenforschung

7-2-2 Eberhard Umbach 外国人運営顧問

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

27 February – 2 March, 2018

This was the first visit with the mission to become acquainted with the entire institute and to focus on the Department of Photo-Molecular Science and the Research Facilities, UVSOR Synchrotron Facility and Center for Mesoscopic Sciences.

General impression:

The overall impression of the IMS was excellent: a research institute of high scientific quality on international scales, with an on average relatively young team of principal investigators (PI, *i.e.* professors and associate professors), well equipped with mostly state-of-the-art instrumentation, highly visible in the international community and well connected and cooperating with leading research groups world-wide. Consequently, the scientific results are well received, highly appreciated, and hence frequently cited by the international community in the research fields covered by IMS.

A closer look into the list of publications reveals that the overall quality is very high, as judged by some recent examples (checked by the reviewer), proven by the percentage of highly ranked publications within the last two years (about one quarter), and corroborated by the top results of national and international citation indices (resulting from past performances). However, the number of peer-reviewed (ISI) publications per year and division (or per PI) is relatively low (5-6/a) compared to similar research institutions world-wide. This is mostly due to the fact that the research groups at IMS are relatively small on average, in particular because some of them do not have graduate students. Thus, the absolute number of graduate students at IMS is relatively small, not even as large as the number of professors (PIs). Of course, this is due to the specific situation of a non-university research institute and probably difficult to change, but efforts and incentives to increase this number could help to support the missions, such as educating young scientists, making more use of the very good infrastructure, and increasing the output.

IMS is one of the five national institutes of natural sciences with the mission of doing fundamental research of high quality in the field of molecular science. This is perfectly fulfilled by the activities of the present research groups. The selected fields covered by the PIs are topical research areas on international scales, some even at the forefront. The frame conditions of a non-university research institute, namely to allow “large-scale research” (involving long time scales, big or complex experiments, high quality technical infrastructure and personnel, *etc.*), are well used by most of the PIs thus perfectly fulfilling the mission of a national research institute. In this context it is highly appreciated that some groups work on topics that require many new developments, high precision and skills, and hence a large amount of endurance, although they may not result in many short-term publications and hence immediate success.

In spite of the mission of IMS to perform fundamental research it is evidently of considerable advantage if some research activities lead to patents, applications, or to successful cooperation with industry. This is not only for giving tax payers and politicians arguments why basic research is useful for society apart from the generation of basic knowledge and education. It also helps to provide motivation and the “arc of suspense” between fundamental questions and “real life” applications. The number of existing good such examples at IMS could be extended, perhaps by suitable incentives.

In addition to these more general remarks, some specific comments are added concerning the above mentioned department and research facilities.

Department of Photo-Molecular Science:

Although the name of this department sounds a bit strange at first glance it makes sense to bundle all fundamental research on molecules interacting with photons in one department because the related topics have several basic aspects in common. Nevertheless the department spans a wide range of interactions of photons with matter including a wide range of wave lengths (infrared to x-rays), time scales (attoseconds to continuous), length scales (single atoms to solid state), and of course research questions. The diversity of the selected topics is high in order to cover a significant range of different issues. It ranges from Laser research (fundamental quantum physics, ultrafast lasers, development of high-power micro-lasers) over nano-optical research for instance in chiral nano-systems over all-parameter band structure investigations on highly correlated materials to investigations on inner- and intermolecular interaction in various liquids and functional organic layers and interfaces. Although the various fields appear significantly different from each other, in at least one case coherence is achieved by adjacent, complementary research fields in order to make best use of the large infrastructure UVSOR. Altogether, the past strategy to set up a department around photon-matter interaction was apparently very successful. Nevertheless, for future hiring processes and infrastructure decisions a careful further development of the strategy appears adequate.

The quality of the research groups as judged from the written reports, from the publications and from the presentations given during the visit can be stated as very high comparing the research groups of this department with similar groups around the world. The attempt to achieve the deepest possible understanding and the very careful investigation of all details and parameters is a common "trade-mark" of this department which is highly appreciated. Several high quality publications and the received international recognition underline this statement. Nevertheless, the output, especially the number of ISI publications per research group (PI) and year, is quite different: it ranges from one to about 10 publications. Although, quality is much more important than quantity, and although the research fields are very different, an enhancement of output in terms of publications in peer-reviewed journals is recommended in some cases.

Professor Ohmori Group:

The visit of the Laser laboratory of K. Ohmori and his team was also very impressive. There are just a few laboratories around the world that have instrumentation of this quality and the scientific potential for studies of quantum states of matter using trapped ultracold atoms and molecules. It is a good choice and nevertheless a great challenge to study the long-range interaction between Rydberg atoms in lattices of three dimensions with attosecond time resolution. There are several fundamental questions that can be answered by such experiments, and once studies of three-dimensional lattices of Rydberg atoms become routine, several new findings for instance concerning collective excitations, surface phenomena, and topological effects in such very weakly interacting "solids" are expected to be accessible.

UVSOR Synchrotron Facility:

UVSOR is a 750 MeV synchrotron radiation (SR) facility of second generation which has very successfully been upgraded in two stages to a competitive, quasi third generation SR source with high brilliance due to a rather low emittance (15 nm-rad). Because of its low primary energy it is dedicated to the UV- and soft x-ray range and because of its low emittance and its 6 undulators it is competitive to all other synchrotron sources in this energy range world-wide. Of course, higher energy synchrotron sources (3 GeV and more) can also cover the low photon energy range, and longer undulators and lower emittance at higher electron energy can provide much higher photon flux densities, but many experiments do not need such high flux densities or the hence possible energy or time resolution. In such cases the availability of a source like UVSOR has several advantages, not least much lower overall costs per experiment. Nevertheless, a careful consideration of the pros and cons as well as a convincing future scientific concept as well as a sufficiently large and effective user community appear necessary if further upgrades and major investments are taken into consideration.

In the past and present N. Kosugi (chair and experiments) and M. Katoh (machine) and their teams have done a marvelous job. With limited resources (as compared to other SR facilities) they have done much refurbishment and many improvements, have achieved an optimum of resulting SR power and research results per time and money within the given boundary conditions; nevertheless still many old components can cause and have caused troubles and need to be replaced. Performance of machine and instruments as well as the obtained scientific results deserve admiration and have significantly contributed to the international visibility of IMS.

Center for Mesoscopic Sciences:

The newly founded Center for Mesoscopic Sciences addresses a field of increasing importance: the mesoscopic “world” covers the range between the fundamental “bricks” atoms and molecules and the macroscopic ensembles like solids and liquids. On mesoscopic scales the size of the systems often plays a decisive role, and properties largely depend on length scales and the number of microscopic elements. Mesoscopic systems are hence scientifically interesting, may require new approaches and may lead to new applications.

Several activities of existing research groups of IMS can be considered to belong to mesoscopic science; others may also contribute to this Center by slight changes of their research program. At present, however only a few research groups are integrated in this Center.

The tour through H. Okamoto’s laboratory for nano-optical investigations was also impressive and yielded a convincing idea of what mesoscopic research for instance could mean at IMS. The further development of this Center, the participation of other research groups with mesoscopic topics, and perhaps some structural clarification could stimulate the success and visibility of this new center.

Conclusion: IMS is a leading research institute with convincing national mission and high international visibility, which has a very good infrastructure and a high research performance. The visit was very interesting and enjoyable, also due to the high professionality and great hospitality of IMS members.

Eberhard Umbach
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Theilheim, March 11th, 2018