7．点検評価と課題

2017年度よりHrvoje Petek教授（ピッツバーグ大学）と中嶋 敦教授（慶應義塾大学）を研究顧問としてお招きし，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。

2018年11月にはマックスプランク研究所（石炭科学研究所）のBenjamin List教授より生命・錯体分子科学研究領域を中心にヒアリングが実施され，グループの研究内容の評価をいただいた。2018年11月にはヴュルツブルク大学のEberhard Umbach名誉教授により，光分子科学研究領域，UVSOR施設，および昨年度設置されたメゾスコピック計測研究センターを中心にヒアリングが実施され，それぞれの研究内容の評価および活動の評価をいただいた。

（川合眞紀）

7-1　外国人運営顧問による点検評価

7-1-1　Eberhard Umbach 外国人運営顧問

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

10 November – 16 November, 2018

The second visit was dedicated to get further insight into the IMS and its research fields, to review in more detail the Departments of Materials Molecular Science and of Theoretical and Computational Molecular Science, and to give advice on the strategical development, in particular the development of large facilities, research directions, co-operations, internal cross-linkings, *etc*.

General impression:

The overall impression of the IMS was again excellent. The remarks of the previous (first) report are of course still valid, especially those about the highly motivated and successful principal investigators, which are relatively young on average, the very interesting and versatile mix of topical research fields, the relatively low number, but high quality of publications, and the relatively small number of graduate students. The present report will focus on strategical aspects.

Large facilities (especially UVSOR Synchrotron Facility):

The justification for the existence of a national institute as compared to research institutes at universities is usually either a research field of national importance (like energy or cancer research) or large-scale science. “Large-scale” means: Large research instruments (like observatories or synchrotron sources), research on long time scales, and research requiring extensive infrastructure, for instance very well equipped laboratories and specialized technical personnel; this all requires relatively large budgets. The mentioned aspects can make national institutes unique and should position them outside direct competition with university groups. For IMS the major justification could be large-scales, apart from the necessity to do internationally highly visible and qualitatively outstanding research in various fields (of molecular science).

Against this background it is strategically important to have, *e.g.*, a Center for Mesoscopic Sciences, a Research Center of Integrative Molecular Systems, or the newly established Exploratory Research Center on Life and Living Systems, ExCELLS. The strategic advantage of such structures is the bundling and focusing of research efforts on selected fields of topical interest by close co-operation across departments within IMS and with best fitting partners outside the institute. In this way, a critical mass can much faster be achieved, research funding can easier be acquired, recruiting of top personnel is facilitated, and national or international visibility are much better obtainable (provided some corporate identity rules are followed).

Strategically even more important is the existence of one or a few large research machine like UVSOR, which not only serves as specialized experimental source for several research groups within IMS but also provides unique research opportunities for users from outside, especially from universities. The challenge, however, is to cope with relatively high costs, for investments as well as for operation. The challenge becomes the larger the older the facility. In such a situation is UVSOR at present, although it is all together in a very good shape and highly successful in operation. A discussion and decision about the different options for the future appears nevertheless appropriate.

There are essentially three main options: a) keep it running with some improvements until its time is up and the repair times and costs make a further operation uneconomic. This could continue for 10–15, perhaps even for 15–20 years (“keep-going” option). b) Plan to shut it down after a fixed period (*e.g.* 10 years) and invest only the absolute necessary repairs and replacements (“phase-out” option). c) Consider a major upgrade for the future which could mean a new, dedicated building, a new storage ring, with new injection system suited for top-up mode, new insertion devices and refurbished end-stations. This would require a lot of money and some time (“boost” option).

Some comparing remarks:

Option b) allows planning of new activities, to set up a new strategic development, to introduce major changes to IMS, and to strengthen selected fashionable fields. However, the existing research with focus on synchrotron radiation (SR)-based methods would then be discouraged; several of the respective group leaders are relatively young and would lose their main methods and hence their motivation. Moreover, such a decision would contradict some recent new employments of group leaders; it should in any case be made before a successor of Prof. Katoh is going to be searched.

Option c) is a difficult decision that cannot be made immediately because it requires some “homework” to be done before. First, a new SR source needs a “scientific case,” *i.e.* a clear concept which science should be made possible, which scientific user communities can be addressed, where it would positioned within the Japanese (and worldwide) SR landscape, which parameters are hence required, and which financial and other resources might be needed. This first exploratory phase would probably last more than a year. The most important point would be a strongly committed, clearly defined user community inside and particularly outside IMS. Secondly, additional money would be needed. For this, the new concept has to be discussed with the decisive authorities, and these must be convinced that this option deserves the extra-money needed. This option would also require a different hiring strategy and long term planning of IMS.

Option a) is the least risky, “continue as is” strategy which does not require major activities now and can be adjusted according to the general development, the upcoming wishes and needs, and the amount of available money.

Further comparisons: Option a) leaves sufficient room for future major strategic changes, while option c) might result in a (major) strategic decision for a new SR source (which leaves nearly no room for other (large) decisions) and option b) would most likely require a new strategic development of IMS. Since an institute like IMS should have some large-scale projects that should not be done by universities it is recommended in case of option b) (and perhaps a) to think about such projects (*e.g.* electron microscopy center with highest resolution and/or cryo-options and/or high throughput; or NMR center for different applications with highest resolution (very high field); or Free Electron Laser; *etc.*). It is further recommended, to base the decision also on the needs of the various other communities within IMS (*e.g.* biology, complex chemistry, material science) and on the wishes of the surrounding universities, institutes, and perhaps even industrial labs. Moreover, if option b) is chosen it should be kept in mind that a severe switch of strategy changes the national and international standing and reputation of IMS with the risk that the existing reputation in the field of SR research gets lost much faster than the international reputation in a new field can be established. In any case, the decision is not easy because it strongly determines the future of IMS and puts much tension on people and resources.

Department of Materials Molecular Science:

Prof. Yokoyama briefly introduced his colleagues in this department and their work (one slide each). Then, he himself as well as Profs. Hiramoto and Kobayashi gave more detailed insight in their research fields and recent results.

The groups of this department cover a wide field of molecular materials research, ranging from the synthesis of molecules with tailored properties (Suzuki), over the tuning of organic semiconductors by targeted and well-controlled doping (Hiramoto) to the development of novel electrochemical devices with solid, H-conducting electrolytes (Kobayashi). Much work is dedicated to the characterization of molecular materials and interfaces under operational conditions, *e.g.* with ambient pressure x-ray photoelectron spectroscopy (Yokoyama) or with sum-frequency generation spectroscopy (Sugimoto), the study of functional molecular materials with various magnetic resonance techniques (Nakamura), the structural and functional characterization of complex molecular assemblies by solid-state NMR (Nishimura), and the detailed, *e.g.* band-structure, study of unconventional properties (superconductivity, Mott-insulator) of organic electronic materials (Yamamoto). The more detailed presentations by Profs. Yokoyama, Hiramoto, and Kobayashi were impressive, because they demonstrated sophisticated approaches under extreme conditions (high pressure, very low doping levels) or with careful analysis of structural information in combination with transport measurements (Kobayashi).

The performance (results, publications) of some of the group leaders appeared to be very good, but there seemed to be nearly no overlap and co-operation between the various groups within the department and with groups in other departments.

Department of Theoretical and Computational Molecular Science:

Prof. Saito carefully introduced this department, his colleagues and their work with about three slides from each group. Then Profs. Ehara, Fujita, and Ishizaki presented their research and discussed recent results in more detail.

These presentations gave the impression of a young, dynamic, and coherent department, working at the forefront of research in well-defined fields. The grouping in three subfields is convincing, at least the distinction between electronic structure and dynamics is obvious and very meaningful (the distinction between quantum and molecular dynamics became less clear).

The investigations of the *electronic structure* cover a variety of important and topical fields, for instance catalysis with very interesting alloy effects in bimetallic nanoclusters and the influence of site effects on selected chemical reactions, or the work on the influences of solvent effects or high pressure on optically excited molecular states, or the quantitative description of chiro-optical spectroscopy by a detailed analysis of the various contributions (Ehara group), or for example the study of exciton quantum dynamics in organic thin films or the calculations of excited states at organic/organic interfaces with long range effects (Fujita).

The investigations of *dynamical properties* in complex systems elucidate the interrelation of structure, dynamics, and function, an important field in particular for biological systems and life science. Topical questions like the heterogeneous dynamics in enzymatic reactions, reactions and fluctuations at single-molecular level and their influence on macroscopic properties, the rhythm mechanism of a clock protein, or the anomalous properties of water are addressed by the Saito group. The Okazaki group concentrates on the question how biomolecular machines work using computational methods; such questions comprise the operation principles of motor

and transport proteins. The Okumura group investigates, for example, the mechanism of the formation of amyloid fibrils by molecular dynamics simulations which may be important to understand the origin of some diseases. And finally the Ishizaki group addresses the fundamental question how to describe best by theoretical methods the chemical dynamics of condensed phases in order to understand, for instance, the energy and charge transport in biological or materials systems, the dynamic fluctuations induced by protein dynamics, the rate of photosynthetic energy transfer including the primary charge separation process, the influence and description of the numerous vibrational modes in complex systems, and the important role of dephasing. Of course, such descriptions can also be used to analyze the charge separation (and recombination) processes in organic photovoltaics.

This department appears rather homogeneous, and there is apparently very good co-operation with other groups, especially with groups in the Department of Life and Coordination-Complex Molecular Science and with groups in Japan and other countries. It remained unclear whether there is any co-operation with groups in the other (experimental) departments of IMS although there seems to be some overlap (*e.g.* excitons or transport). Moreover, many of the other experimental groups could much profit from in-house theory which complements (some of) their research fields such that more fruitful collaboration within IMS would be possible. Future recruitment could take care of this aspect.

Other Departments and Activities:

This visit concentrated on the two above-discussed departments. However, two overview presentations on the Department of Photo-Molecular Science and on the Department of Life and Coordination-Complex Molecular Science completed the overview of IMS. Especially the introduction by Prof. Iino gave a very clear and comprehensive insight into the activities of the latter department because he presented not only his work in some detail but also high-lighted the work of his colleagues such that a very interesting and coherent picture of this department emerged.

In addition, Prof. Ohmori gave new information about recent results from the groups of the Department of Photo-Molecular Science, especially exiting news from his own research. Prof. Kera discussed his thoughts about the future development of UVSOR, and Dr. Matsui gave an impressive overview on his former achievements which are planned to result in the development of a next generation momentum microscope for UVSOR. This could nicely complement the instrumentation at this synchrotron source utilizing the specific properties of UVSOR and making it more competitive on international scales.

Right at the beginning of the visit, the new activity ExCELLS which was already mentioned above was introduced by Prof. Kato. He could impressively demonstrate which fields will be addressed by this new center and how cross-institutional co-operation will be utilized to tackle topical questions in life science. This center addresses the central question of what is the basis of life, for example how structure, dynamics, and function interdepend, how molecular self-assembly and dynamic processes create function, and how selected (bio)molecular systems actually operate. The foundation of ExCELLS and the integration of various research groups from different institutes will certainly enhance interdisciplinary and inter-institutional co-operation, may result in better access to new research projects including additional research money, could enable experiments under extreme conditions (deep water, outer space), and should considerably increase the national and international visibility.

Co-operation:

The internal co-operation is partly excellent, partly fine and partly lacking. Excellent is, for example, the cooperation between many groups of the Department of Life and Coordination-Complex Molecular Science and the Department of Theoretical and Computational Molecular Science, as mentioned above. On the other side of the spectrum is the (non-existing) cooperation between some groups within the Departments of Photo-Molecular Science and Materials Molecular Science and between these and other groups of IMS. Of course, in an institute of the versatility of IMS many groups do not have sufficient overlap with each other and hence have no common denominator for co-operation. However, some more collaborative activities in particular between the non-bio groups could create added value and more visibility from outside.

Co-operation of IMS groups with groups outside IMS is partly very good and partly hardly existing. Some groups have intensive contacts with other groups in Japan, they also preferentially cite groups in Japan, and they orient themselves along the developments within Japan. Although this is very well understandable because Japan is the most important "market" for them, more contacts on international scales would be highly desirable because the international science scene finally sets the milestones and success measures. And of course a national institute like IMS should be highly visible on international scales. It is clear that this impression is not valid for all groups, because some have excellent international relations and co-operations and hence contribute to the mentioned, very good international standing of IMS. But for other groups there is considerable room for improvement.

Some further structural aspects:

The (honorable) departure of two group leaders from the Center for Mesoscopic Sciences as well as the two vacancies within the Department of Theoretical and Computational Molecular Science allow some re-structuring. While the latter vacancies could be used to enable more co-operation between theory and experiment in other fields than those which already co-operate (see above), the former could be taken as chance to develop a new concept for Laser research. Perhaps this chance could also be used to restructure the rather heterogeneous Department of Photo-Molecular Science and the Center for Mesoscopic Sciences. Of course, depending on the decision on the future of UVSOR (see above) more overlap between synchrotron research and other fields of research within IMS could be generated by proper selection of new research groups. Also a strengthening of the (presently reduced) Laser activities perhaps in connection with mesoscopic or nanoscopic science would make sense. Moreover, for new recruitments two more aspects should be seriously considered: To increase the number of female principal investigators and to hire persons from other countries to make IMS more international.

Conclusion:

IMS is an excellent research institute with a convincing national mission and very good international visibility in several fields; it has a valuable infrastructure and a high research performance. Also the second visit was very interesting and enjoyable, due to the high professionality and great hospitality of IMS members.

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