7-2　光分子科学研究領域の評価

7-2-1　Matthias Weidemüller 外国人運営顧問

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

22 March to 27 March 2023

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

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

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

General remarks

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

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

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

UVSOR Synchrotron Facility and associated research groups

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

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

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

Masahiro KATOH

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

Fumihiko MATSUI

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

Kiyohisa TANAKA

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

Yoshitaka TAIRA

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

Research groups from the Department of Photo-Molecular Science

Kenji OHMORI

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

Hiromi OKAMOTO

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

Satoshi KERA

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

Research group from the Department of Materials Molecular Science

Toshiki SUGIMOTO

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

Research group from the Research Center of Integrative Molecular Systems

Hikaru KURAMOCHI

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

Research group from the Center for Mesoscopic Sciences

Takahashi KUMAGAI

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

Research group from the Division of Research Innovation and Collaboration

Takunori TAIRA

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

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

Heidelberg, 30 April 2023