Institute for Molecular Science (IMS) is one of the world’s core research facilities for molecular science and is also a center for inter-university joint research in Japan. It sets an extremely wide range of research goals, from understanding the behavior of individual molecules to that of collective molecular systems. These molecular systems have close relation to scientific understanding of biology, engineering and space sciences. Currently, IMS is engaged in six (four plus two) areas of research: Theoretical and computational molecular science, Photo-molecular science, Materials molecular science, and Life and coordination-complex molecular science. Research Center of Integrative Molecular Systems (CIMoS) has started from April 2013 to develop the highly functional molecular systems such as molecular rhythms, sensing and response, and even self-repair. Starting from April 2017, Center for Mesoscopic Sciences (CMS) is launched to develop innovative methodology of studying mesoscopic molecular systems, covering from theoretical methods to leading-edge measurement methods. Division of Advanced Molecular Science is launched to promote outstanding research example of Molecular Science from April 2018. From April 2019, Division of Research Innovation and Collaboration is launched to strengthen the tie between the social activities. In addition to these research divisions, IMS has three research facilities; UVSOR Synchrotron Facility, Instrument Center facilitated with various molecular detectors, and Equipment Development Center. IMS also operates the Research Center for Computational Science, jointly with National Institute for Physiological Sciences and National Institute for Basic Biology in the same campus. From April 2018, Exploratory Research Center on Life and Living Systems (ExCEILS) is launched directly under the National Institutes of Natural Sciences to advance the activity of Okazaki Institute for Integrative Bioscience (OIIIB).

Annual Review 2021 is a summary of research activities performed in IMS during September 2020–September 2021. Individual research groups at IMS are making steady progress in basic research on molecular structures, reactions and functions demonstrating “novel molecular capabilities,” as reported in this Review. In addition to these individual activities, IMS conducts the six special programs in the institute basis: (i) Development of cold-atom based quantum simulators and their applications to quantum computing within the framework of Japan’s flagship program on quantum sciences and technologies “Q-LEAP” by MEXT (2018–2028); (ii) Nano science project, called Nanotechnology Platform; (iii) Advanced Research Infrastructure for Materials and Nanotechnology in Japan, from April 2021; (iv) Inter-University Network for Common Utilization of Research Equipments; (v) Project on trans-hierarchical studies of materials and biological systems with molecular observations, as a joint program of NINS; (vi) IMS runs several international collaboration programs and also owns an internship program for young scientists: Institute for Molecular Science International Internship Program (IMS-IIP). IMS-IIP provides the opportunity of internship for young researchers (e.g., master’s and doctoral students, postdoctoral researchers and young faculty members of MOU partners) from overseas to stay in IMS laboratories.

Our life in Okazaki has changed since April 2020 due to the pandemic of COVID19. Utilization of WEB meeting has become the standard for most of the academic meetings and thus the opportunity to meet and discuss with our colleague all around the world has become easier than ever. Unexpected findings by directly encountering people face to face is no more an everyday life. Accepting Post-Docs and students from outside Japan is extremely difficult. Experimental collaboration based on practical exchange of personal has been restricted, while some new idea to perform the experiment by accepting samples from the users has started this year. From the administration point of view, acceleration of reforming our work style such as work from home has been realized, accompanied with paperless meeting and digitalization of office documents. Such a revolution is still ongoing while the most impressive change was getting rid of our sealing culture in a part.

IMS will continue to contribute to lead the Molecular Science together with many young promising and well-established senior scientists. This institute has been most benefited with your constant support and we do expect your further support and advice for creating this new era of molecular science.

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KAWAI, Maki
Director General, Institute for Molecular Science