



This Annual Review 2012 is a summary of research activities performed in the Institute for Molecular Science (IMS) during September 2011–August 2012. IMS is one of the world's core research facilities for molecular science and is a center for inter-university joint research in Japan, as well. It sets an extremely wide range of research goals, from understanding the behavior of individual molecules to that of collective molecular processes on the scale of life forms and in space. Currently, the IMS is engaged in four areas of research: Theoretical and computational molecular science, photo-molecular science, materials molecular science and life and coordination-complex molecular science. It operates seven research facilities, including the UVSOR Facility.

The staff 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 research activities, IMS conducts the six special programs in the institute basis; (i) Two computational chemistry programs: TCCI (Theoretical and Computational Chemistry Initiative) as a part of CMSI (Computational Materials Science Initiative) in HPCI (High Performance Computational Infra), and Nano-science simulation for the “Grand Challenge Applications” of the next generation supercomputer projects (the latter was till March 2012), (ii) Nano-network project, including the joint research initiative using 920MHz NMR, (iii) Extreme photonics in collaboration with RIKEN, (iv) COE of molecular and materials simulations as a joint program of NINS, (v) Quantum Beam Development Program in collaboration with Kyoto University and Nagoya University, and (vi) Networked Laboratories for the Frontiers of Photon Science and Technology in collaboration with Japan Atomic Energy Research Institute, Osaka University and Kyoto University. With two IMS own international programs for Asia, namely, EXODASS (EXchange prOgram for the Development of Asian Scientific Society) and Asian Core, IMS has invited active young scientists from various East Asian countries to carry out collaborative researches. EXODASS Program is the post-JENESYS starting from 2011, aims to provide the opportunity for young researchers (*e.g.*, master's and doctoral students and postdoctoral researchers) from Asian countries to stay in IMS laboratories related to the basic research for environmental and energy problems. Asian Core programs now also becomes IMS own project and continue to strengthen the tie among the four key institutes of Chemical Physics in Asia, namely, KAIST in Korea, IASM in Taiwan, ICCAS in China and IMS in Japan.

Three professors, Professor Tanaka, Professor Nagase, and Professor Hirata, are retired at the end of March 2012 and now become our emeritus professors. Two associate professors, Professor Yonemitsu and Professor Mitsuke, were promoted to full professors of Chuo and Josai Universities, respectively. We are grateful to all five professors for their great contribution to IMS. As for our new faculty, five new members have joined to the our faculty. Dr. Akiyama, an expert of biomolecular systems, and Dr. Murahashi, an organometallic chemist, and Dr. Yamamoto, a solid-state chemist, becomes our full professors. Two young theoretical chemical physicists, Dr. Ishizaki and Dr. Shikano have joined us as the independent young researchers (of new associate professor positions).

IMS is continuing to employ a new scientific perspective to examine the boundary between “micro” and “macro” phenomena, which is “an intrinsic arena for the generation of life” and “for the evolution of functioning molecular materials.” We do expect your advice and support for creating this new era of molecular science.

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OHMINE, Iwao
Director-General, Institute for Molecular Science