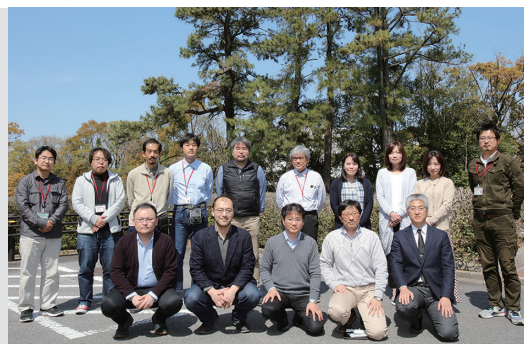


Research Center for Computational Science (Okazaki Research Facilities)

EHARA, Masahiro	Director, Professor
SAITO, Shinji	Professor
OKUMURA, Hisashi	Associate Professor
OKAZAKI, Kei-ichi	Associate Professor
OONO, Hitoshi	Associate Professor
UCHIYAMA, Ikuro	Associate Professor
ISHIDA, Tateki	Assistant Professor
IWAHASHI, Kensuke	Chief Engineer (Unit Leader)
MIZUTANI, Fumiyasu	Engineer
NAITO, Shigeki	Chief Technician
KAMIYA, Motoshi	Chief Technician
SAWA, Masataka	Technician
NAGAYA, Takakazu	Technician
KINOSHITA, Takamasa	Technician
YAZAKI, Toshiko	Technical Fellow
UNO, Akiko	Technical Fellow
KONDO, Naoko	Secretary
KONDO, Noriko	Secretary
URANO, Hiroko	Secretary



Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* solid state physics, biophysics, and physiology. Our systems consist of NEC LX (406Rh-2, 110-Rh1, 108Th-4G; since Oct. 2017). The NEC LX 406Rh-2 and 110-Rh1 combined system, named “Molecular Simulator,” is ranked 261st position in the TOP500 supercomputer list in June 2020. These massive computer resources have been used for various kinds of large-scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods. We also provide a number of application programs to the users: Gaussian, GAMESS, Molpro, AMBER, Gromacs, and so on. The supercomputer systems had been used by 1,142 researchers from 271 groups in fiscal year 2020. Some of the computational resources are provided to the following projects: Program for Promoting Research on the Supercomputer Fugaku, Professional development Consortium for Computational Materials Scientists (PCoMS), and Elementary Strategy Initiative to Form a Core Research Center.

For fostering young generation, we organize the schools of quantum chemistry and molecular dynamics simulation every year. We also organize the RCCS supercomputer workshop focusing on the new trends of computational chemistry for the purpose of the research exchange and human resource development.

We organized a joint Supercomputer workshop of the Research Center for Computational Science and the Nano-technology Platform Project, “Toward Collaboration between Theoretical/Computational Science and Experimental Science Based on Data Science” and two schools “The 10th Quantum Chemistry School” and “The 14th Molecular Simulation School—From Basics to Applications. In cooperation with Institute for Materials Research, Tohoku University, Institute for Solid State Physics, University of Tokyo, and Nanoscience Design Center, Osaka University, we established the Council for Computational

Materials Science to promote the cutting-edge computational materials science technology of Japan, to create world-class results, and to realize the social implementation of simulation technology and materials information science technology.

We also offer Quantum Chemistry Literature Database (QCLDB; <http://qcldb2.ims.ac.jp/>), Force Constant Database (FCDB; <http://fcdb.ims.ac.jp/>), and Segmented Gaussian Basis Set (SGBS; <http://sapporo.center.ims.ac.jp/sapporo/>) services. The latest release, QCLDB II Release 2016, containing 139,657 data of quantum chemical studies is available for the registered users. FCDB provides force constants of molecules collected from literature. SGBS service provides basis sets for atoms which efficiently incorporate valence and core electron correlations (also known as Sapporo basis sets) in various quantum chemistry package formats. Further details about the hardware, software, and the other services are available on our website (English: <https://ccportal.ims.ac.jp/en/>, Japanese: <https://ccportal.ims.ac.jp/>).

The center is jointly managed with National Institute for Physiological Sciences and National Institute for Basic Biology (both in the same campus).



Figure 1. NEC LX.