

# Research Center for Computational Science (Okazaki Research Facilities)

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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, basic biology, and physiology. Our systems consist of HPE Apollo 2000 and Apollo 6500 (since Feb. 2023). The combined system, named “Molecular Simulator,” is ranked 196<sup>th</sup> position in the TOP500 supercomputer list in June 2023. 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 about 30 application programs to the users: Gaussian, GAMESS, Molpro, AMBER, Gromacs, and so on. In particular, we have implemented some original programs developed by researchers in Japan to provide them to the users. The supercomputer systems had been used by 1,315 researchers from 302 groups in the fiscal year 2023. 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. In the fiscal year 2023, the numbers of registered attendants of these schools were 329 and 380, respectively. 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. In the fiscal year 2023, we organized the workshop under the title, “Frontiers of Biomolecular Science based on Simulations, Informatics, and AI.”

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 Computational Materials Science Forum

(CMSF) 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://fcd.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.** HPE Apollo 2000 and Apollo 6500.