Research Center for Computational Science

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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 and biophysics. The computer systems consist of Fujitsu PRIMERGY RX300, PRIME HPC FX10 and PRIMERGY CX2550, SGI UV2000. The systems have been used by 813 people in 221 research groups in 2016. Large scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods, have been performed with the systems. The Center also provides a number of application programs, for example Gaussian 09, GAMESS, Molpro, AMBER, and NAMD. The Center offers the Quantum Chemistry Literature Database, which has been developed by the Quantum Chemistry Database Group in collaboration with members of the Center. The latest release, QCLDB II Release 2016, contains 139,657 data of quantum chemical studies. Detailed information on the hardware and software is available on the web site (http://ccportal.ims.ac.jp/).

In addition to the provision of computational resources to individual academic researchers in Japan, the Center contributes up to 20% of the computational resources to the Post-K Supercomputer Priority Researches 5 and 7 and the Professional development Consortium for Computational Materials Scientists.

Figure 1. Fujitsu PRIMERGY CX2550.

Figure 2. SGI UV2000.