## Materials Design and Characterization Laboratory (MDCL)

The MDCL was established as the third research facility of the Institute for Solid State Physics (ISSP) when the latter was reorganized in May 1996. Its aim is to promote material science with an emphasis on the "DSC cycle", where DSC stands for design, synthesis and characterization, three processes for developing new materials.

The MDCL consists of two sections, Materials Design (MD) section and Materials Synthesis and Characterization (MSC) section. The Supercomputer Center of the ISSP (SCC-ISSP) is placed in the MD section, while in the MSC section there are seven laboratories for joint use; Materials Synthesis Laboratory, Chemical Analysis Laboratory, X-ray Diffraction Laboratory, Electron Microscope Laboratory, Electromagnetic Measurement Laboratory, Spectroscopy Laboratory, and High-Pressure Synthesis Laboratory.

Almost all the facilities of the MDCL are open to scientists in Japan through the User Programs conducted by two steering committees of the MDCL. One is the steering committee of the SCC-ISSP, under which the Supercomputer Project Advisory Committee is placed for reviewing proposals. The other is the steering committee of the MSC facilities. More than half of the members of these committees are from the outside of ISSP.

## COVER FIGURE

Conformation of an ultra-long chain fatty acid, dTSPC, in DSPC bilayer. The dTSPC molecule is represented by colored spheres.

See Page 35–43, K. Kawaguchi and H. Noguchi, "Molecular dynamics study of ultra-long chain fatty acid in lipid bilayer".

# PREFACE

The Supercomputer Center (SCC) is a part of the Materials Design and Characterization Laboratory (MDCL) of ISSP. Its mission is to serve the whole community of computational condensed-matter physics of Japan providing it with high performance computing environment. In particular, the SCC selectively promotes and supports large-scale computations. For this purpose, the SCC invites proposals for supercomputer-aided research projects and hosts the Steering Committee, as mentioned below, that evaluates the proposals.

The ISSP supercomputer system consists of two subsystems: System B, which was last replaced in Oct. 2020, is intended for larger total computational power and has more nodes with relatively loose connections whereas System C is intended for higher communication speed among nodes. System B (ohtaka) consists of 1680 CPU nodes of AMD EPYC 7702 (64 cores) and 8 FAT nodes of Intel Xeon Platinum 8280 (28 cores) with total theoretical performance of 6.881 PFlops. System C was replaced in June 2022 and the current system (kugui) consists of 128 CPU nodes of AMD EPYC 7763 (64 cores) and 8 ACC nodes of AMD EPYC 7763 (64 cores) NVIDIA A100 40GB for HGX with total theoretical performance of 0.973 PFLOPS.

In addition to the hardware administration, the SCC puts increasing effort on the software support. Since 2015, the SCC has been conducting “Project for advancement of software usability in materials science (PASUMS).” In this project, for enhancing the usability of the ISSP supercomputer system, we conduct several software-advancement activities: developing new application software that runs efficiently on the ISSP supercomputer system, adding new functions to existing codes, help releasing private codes for public use, creating/improving manuals for public codes, etc. Two target programs were selected for fiscal year 2022: (1) abICS (proposal made by S. Kasamatsu (Yamagata U.)), and (2) H-wave (proposal made by A. Kobayashi (Nagoya U.)). In addition, since 2021, we have been maintaining the data repository service for secure storage and enhanced usability of results of numerical calculation.

All staff members of university faculties or public research institutes in Japan are invited to propose research projects (called User Program). The proposals are evaluated by the Steering Committee of SCC. Peer-reviewing is done by the Supercomputer Project Advisory Committee. In fiscal year 2022, totally 337 projects were approved including the ones under the framework of Supercomputing Consortium for Computational Materials Science (SCCMS), which specially supports FUGAKU and other major projects in computational materials science.

The research projects are roughly classified into the following three (the number of projects approved):

First-Principles Calculation of Materials Properties (151)
Strongly Correlated Quantum Systems (25)
Cooperative Phenomena in Complex, Macroscopic Systems (141)

In all the three categories, most proposals involve both methodology and applications. The results of the projects are reported in 'Activity Report 2022' of the SCC. Every year 3-4 projects are selected for “invited papers” and published at the beginning of the Activity Report. In the Activity Report 2022, the following three invited papers are included:

``Training method for refinement of machine-learning interatomic potential and its applications",
Kohei SHIMAMURA, Akihide KOURA, and Fuyuki SHIMOJO (Kumamoto Univ.)

``First principles calculation of copper-oxide superconductors exhibiting electron fractionalization",
Masatoshi IMADA (Waseda Univ.)

``Molecular dynamics study of ultra-long chain fatty acid in lipid bilayer",
Kazutomo KAWAGUCHI (Kanazawa Univ.) and Hiroshi NOGUCHI (ISSP)

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