

## **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**

Stable 6x6 surface structure obtained by Bayesian optimization. Brown, blue and white atoms correspond to Ga, N and H, respectively.

See Page 42–44, A. Oshiyama, ”Clarification of Microscopic Mechanisms of Semiconductor Epitaxial Growth and Device-Interface Formation by Large-Scale Quantum-Theory-Based Computations”.

## 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 (enaga) consists of 252 nodes of HPE SGI 8600 with 0.77 PFLOPS, which stopped operation in Dec. 2021 for replacement. The new machine (kugui), which consists of 128 nodes of AMD EPYC 7763 (128 cores) and 8 nodes of AMD EPYC 7763 (64 cores) with total theoretical performance of 0.973 PFLOPS, will start operation in June 2022.

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. Three target programs were selected in fiscal year 2021 and developed or enhanced the usability of software were released as (1) ESM-RISM (proposal made by M. Otani (AIST)), and (2) 2DMAT (proposal made by T. Hoshi (Tottori Univ.)). In 2021, we also started the data repository service for storing results of numerical calculation and enhancing their reusability.

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. Pre-reviewing is done by the Supercomputer Project Advisory Committee. In fiscal year 2021, totally 321 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 (142)
- Strongly Correlated Quantum Systems (29)
- Cooperative Phenomena in Complex, Macroscopic Systems (128)

In all the three categories, most proposals involve both methodology and applications. The results of the projects are reported in 'Activity Report 2021' 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 2021, the following three invited papers are included:

"Theory, practice, and application of the van der Waals density functional",  
Ikutaro HAMADA (Osaka Univ.)

"Development of permanent magnet materials—from the view point of first-principles  
calculation",  
Hisazumi AKAI (ISSP) and Shinji TSUNEYUKI (Univ. Tokyo)

"Development of Bayesian optimization tool and its applications in materials science",  
Ryo TAMURA (NIMS), Yuichi MOTOYAMA (ISSP), and Kazuyoshi YOSHIMI (ISSP)

June 2, 2022

Naoki Kawashima  
(Chairman of the steering committee, SCC, ISSP)

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