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

Crystal structures and phonon properties of thermoelectric clathrate $Ba_8Ga_{16}Ge_{30}$.
Adopted from T. Tadano and S. Tsuneyuki: Phys. Rev. Lett. 120 (2018) 105901.
See T. Tadano, Page 15–24, "First-principles calculation of thermophysical properties of solids with strong phonon anharmonicity".

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 is intended for more nodes with relatively loose connections. In July, 2015, the SCC replaced the two supercomputer subsystems (SGI Altix ICE 8400EX and NEC SX-9) to one new system (System B, SGI ICE XA/UV hybrid system). The system B consists of 1584 CPU nodes, 288 ACC nodes, and 19 FAT nodes. The CPU node has 2 CPUs (Intel Xeon). The ACC node has 2CPUs (Intel Xeon) and 2GPUs (NVIDIA Tesla K40). The FAT node has 4CPUs (Intel Xeon) and large memory (1TB). The system B has totally 2.6 PFlops theoretical peak performance.
The new system C (HPE SGI 8600) was installed in January, 2018. It consists of 252 nodes, and each node has 2 CPUs (Intel Xeon) and 192 GB of memory. The system C has totally 774 TFlops.

The hardware administration is not the only function of the SCC. Since 2015, the SCC has started “Project for advancement of software usability in materials science”. In this project, for enhancing the usability of the ISSP supercomputer system, we perform some software-advancement activities such as implementing a new function to an existing code, releasing a private code on Web, and writing manuals. Two target programs were selected in school year 2019 and developed software were released as abICS (proposal made by S. Kasamatsu (Yamagata Univ.)) and TeNeS (proposal made by N. Kawashima (ISSP)). The SCC has also started a service for porting users’ materials science software to General Purpose GPUs (GPGPU) since 2015. One program was selected for the GPGPU porting in school year 2019.

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 school year 2019, totally 309 projects were approved. The total points applied and approved are listed on Table. 1 below. Additionally, we supported post-K and other computational materials science projects through Supercomputing Consortium for Computational Materials Science (SCCMS).

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

First-Principles Calculation of Materials Properties (145)
Strongly Correlated Quantum Systems (36)
Cooperative Phenomena in Complex, Macroscopic Systems (128)

All the three involve both methodology of computation and its applications. The results of the projects are reported in 'Activity Report 2019' 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 2019, the following three invited papers are included:

"First-Principles Calculation of Thermophysical Properties of Solids with Strong Phonon Anharmonicity",
Terumasa TADANO

"Development of Open-Source Parallelized Tensor Network Softwares: mptensor and TeNeS",
Satoshi MORITA and Naoki KAWASHIMA

"Disorder-Free Glass Transitions of Spins and Orbitals in a Frustrated Pyrochlore Magnet”,
Kota MITSUMOTO, Chisa HOTTA, and Hajime YOSHINO

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Naoki Kawashima
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