Conferences and Workshops

Frontiers of Quantum Computational Science

July 9-10, 2020 H. Shinaoka, T. Okubo, J. Otsuki, N. Kawashima, S. Todo, T. Misawa, and S. Morita

Various numerical methods such as dynamical mean-field approximation, variational Monte Carlo, and tensor network methods have been developed for solving quantum many-body problems. In addition, there are many attempts to quantitatively predict the properties of strongly correlated materials by integrating these elaborate many-body methods and first-principles methods. In recent years, new approaches using machine learning, quantum computers, and quantum chemical methods have emerged for solving many-body problems. There is a need for an opportunity for researchers in different fields to meet, exchange information, and have extensive discussions. The Institute of Solid State Physics has been playing an essential role as a center for computational condensed matter physics. Thus, it is of great significance for the future development of computational condensed matter physics to hold a short-term workshop with experts in these different fields.

In line with the workshop theme, we invited young researchers in quantum computing, machine learning, information theory, and in first-principles and model calculations on quantum many-body systems. The final program consisted of 20 oral talks (including 11 invited talks) and 15 poster talks. The number of registered participants was 180, and more than 150 attended both days, with a maximum of 120 simultaneous participants in realtime. Although the workshop was held online using Webex and Slack due to the COVID-19 pandemic, there were extensive discussions between participants in oral and poster talks.



Present Status of Neutron Scattering Research and the Future Prospect after the Restart of JRR-3

July 27-29, 2020 ato T. Osakabe, M. Sugiyama, and M. Hino

T. Masuda, T. Nakajima, O. Yamamuro, M. Fujita, T. Sato, T. Osakabe, M. Sugiyama, and M. Hino

Neutron Science Laboratory (NSL) operates collaboration research using research reactor JRR-3 and has been leading neutron scattering science. JRR-3, however, has suspended its operation since the Great East Japan Earthquake in 2011. Owing to the strong and patient demand from the neutron science community, JRR-3 has finally restarted in February 2021 after the long aseismic reinforcing work. In prior to the restart, NSL held the ISSP regular workshop for the neutron users to discuss the frontier of the research related to neutron science, for the instrumental scientists to propose possible research plan after the restart, and for both to discuss new institution of collaboration research constructed under the latest safety standard. Because of the COVID19 the workshop was held using ZOOM, and 115 scientists including those from abroad participated. 15 presentations on solid state physics and 15 presentations on material science and soft matter were made followed by active discussions. 5 presentation on the new institution of the collaboration research were made on the last day. NSL director Yamamuro proposed the revised plan of Instrumental scientists as well as the revised proposal format of the general user program meeting the latest safety standard. In spite of the first ZOOM workshop for NSL it finished a success.

Recent Developments and Future Prospects of Quantum Materials Research

September 24, 28, 29, 2020 Y. Otani, M. Yamashita, and Z. Hiroi

Condensed matter physics has evolved significantly through the discovery of new substances, phenomena and concepts. Especially in the strongly correlated electron system field where simple one-particle approximation breaks down, close cooperation of synthesis, measurement, and theory, which bear these three elements, is important. In recent years, quantum materials that have developed strongly correlated electron systems have been attracting attention, and the Institute for Solid State Physics, University of Tokyo has established a quantum materials research group with the aim of breaking through research through the fusion of fields. Furthermore, the experimental group of the Material Design and Characterization Laboratory, which has been responsible for material development, and the Research Division of the Condensed Matter Physics, which has been mainly responsible for measurement, are strongly collaborating with the Quantum Materials Research Group to develop active research.

Based on the above situation, this ISSP workshop focused on material development in quantum materials research and experimental research using various measurement methods, and aimed to give an overview of the current state of recent research and discuss future research prospects. The event was co-sponsored by the Quantum Materials Research Group, the Research Division of the Condensed Matter Physics, and the Material Design and Characterization Laboratory.

The workshop was held in the morning of three days in the form of presentation at Zoom, and a total of 18 researchers gave lectures in the program. Pre-registration reached 171 people, with 120-130 participants daily throughout the three days. The speakers introduced recent research on quantum materials and expressed their opinions on future prospects, and there were many questions and comments from the participants, and lively discussions took place. Although it was held in an unusual format using Zoom, it was as meaningful an opportunity as the conventional workshop. It was also an opportunity to think about the future of the research at the Institute for Solid State Physics.

Computational Materials Science — New Perspectives 2020—

December 21- 22, 2020 O. Sugino, T. Ozaki, N. Kawashima, H. Noguchi, T. Fukushima, Y. Higuchi, S. Morita, J. Haruyama, M. Kawamura, M. Fukuda, and K. Ido

This workshop was organized for the computational condensed matter research community, especially for the users of the ISSP supercomputers, to exchange the most recent information on the computational condensed matter research and on the high-performance computation of related research areas. This was held as a series of annual workshop of ISSP supercomputer that has been held every year. However, the workshop has been postponed from April to December due to the state of emergency caused by COVID-19 and has been held at ONLINE. The registered people were 135. The selected topics include the target of the Fugaku supercomputer project, the emergent data-driven material research, and "Project for advancement of software usability in materials science (PASUMS)" that developed the ab-Initio Configuration Sampling tool kit (abICS) to solve the replica exchange Monte Carlo (RXMC) sampling coupled directly with local structural relaxation and energy calculation using DFT codes in 2019. In addition to 19 invited talks, 26 poster presentations, and a special lecture for data-repository were given by Prof. Miho Funamori. In the poster presentation, short talk presentations and discussions using an online bulletin

board and zoom break-out room have been set. The posters were evaluated by invited speakers and the organizers; three posters were selected and given the poster award.



Present and Future of Data Science in Condensed Matter Physics

K. Yoshimi, T. Ozaki, O. Sugino, H. Noguchi, T. Fukushima, K. Ido, M. Fukuda, R. Tamura, and N. Kawashima

Recently, researchers are becoming more enthusiastic in application of data-scientific methods to condensed matter physics, with the hope for developing a new scheme for numerical simulation, improvement of quality of theoretical predictions, and acceleration in search and development of new materials. From these activities, problems arise concerning how we manage ever-increasing data and make them more usable in the new schemes. We intended this workshop to be an opportunity for the participants to share experience in application of data-scientific methods to condensed matter physics and biochemistry, as well as data-base construction and its maintenance. We had 209 registrations and recorded 150 maximam simultaneous participants on the first day and 120 for the second. The first day was dedicated to the application of machine learning in physics and biochemistry whereas the second day was for data-repositories and data-bases. Concerning application of the machine learning, Sugino (ISSP) gave a presentation on machine learning for basic aspects of the theoretical condensed matter physics, i.e., the numerical estimation of the Kohn-Sham exchange-correlation potential. Ozaki (ISSP), Fukushima (ISSP) and Chikyo (NIMS) presented their works on the comprehensive high-throughput calculation and/or construction of material data-bases. Terayama (Yokohama City U.) discussed the 3D structural study of protein molecules aided by the machine learning, and Inoue (ISSP) talked about function prediction of amino-acid sequences. As for data-repositories and data-bases, Katsura (NIMS) talked about the construction of the data-base from the graphic information of research papers, and its applications. Taura (U Tokyo) presented the current state of the starting project on "mdx". Kobayashi(ISSP)'s talk was about lasor manifacturing as a potential target of data-accumulation and machine-learning. Miyake (AIST) presented their recent result on the data assimilation method based on both numerical and experimental data in search of new magnetic materials. Upon these results, we also held a panel discussion to further discuss what new framework is to be created for the data management and how we should proceed in its applications, with panellers being Kobayashi (ISSP), Tamura (U Tokyo and NIMS), Katsura (NIMS) and Shoji (TOYOTA) and the mediator Yoshimi (ISSP).

Core Technology Toward the Frontier Soft X-Ray Science

March 4, 2021 T. Kimura, T. Arima, F. Komori, Y. Harada, I. Matsuda, H. Mimura, and T Kondo

February 22 and 24, 2021

The workshop was organized on March 4 by the Institute for Solid State Physics (ISSP) and Synchrotron Radiation Research Organization of the University of Tokyo (UTokyo-SRRO) and User Community VUV-SX High-Brilliance Light Sources. The workshop was held online using ZOOM, and about 140 participants from a wide range of fields, including universities, companies and research institutes, attended. In this workshop, eight researchers were invited to give talks on the latest trends in soft X-ray science and to discuss the new direction that will emerge from the next-generation synchrotron radiation facility in Sendai. The next-generation synchrotron radiation facility is expected to improve the coherence and intensity of X-rays. In each lecture, various research results on imaging and spectroscopic techniques were reported, ranging from basic beamline technologies to applied measurements, which can use the features of the new facility. The newly-organized general discussion session (Moderator: Professor Abukawa from Tohoku University) provided an opportunity for in-depth questions and answers about the contents of each lecture. In the last session, Director Harada presented the prospects and direction of the SOR facility towards the operation start of the new synchrotron radiation facility in 2023.





The International Workshop on Quantum Magnets in Extreme Conditions

March 22-26, 2021 Y. Kohama, F. Mila, and M. Jaime

This workshop was hold as an online virtual conference due to the COVID-19 pandemic. The main focus of this workshop was the fascinating emergent physical properties of solid-state quantum magnets in both theoretical and experimental research fields. The workshop was free of charge and started from 21:00 pm to 24:00 pm in JST (13:00 pm - 16:00 pm in CET and 8:00 am - 11:00 am in EDT) to encourage the participation of international students and upcoming international researchers. The total number of registrations was 438. The numbers of participants on Monday, Tuesday, Wednesday, Thursday, and Friday were 320, 234, 221, 179, and 151, respectively (the total number of participants was 1105). The 25 talks were given by the invited speakers who are leading scientists in their field of research. It should be noted that the second international workshop on Quantum Magnets in Extreme Conditions is tentatively scheduled in 2023 as a hybrid conference. We hope that the next workshop can give us a chance to share novel idea and to exchange the forthcoming results in this exciting research fields.

