

# Conferences and Workshops

## The 5th Ito International Research Center Conference “Forefront of Molecular Dynamics at Surfaces and Interfaces: from a Single Molecule to Catalytic Reaction”

November 20 - 23, 2017

J. Yoshinobu

In cooperation with Surface and Interface Spectroscopy Forum in Japan, the present international conference was held from November 20 to 23, 2017 at Ito Hall of The University of Tokyo (Hongo campus), with the financial support of Ito International Academic Research Center Foundation (The University of Tokyo), the RIKEN Centennial Anniversary Project, ISSP International Workshop, and ISSP Workshop. There were 196 participants, including 30 invited speakers, 13 contributed oral presentations and 109 poster presentations (133 participants from Japan including 19 invited speakers and 63 participants from abroad including 15 invited speakers).

Chair of the executive committee was Prof. Jun Yoshinobu (ISSP) and Co-chair was Dr. Kim Yousoo (RIKEN); the other committee members were Prof. Shigeru Masuda (The University of Tokyo), Prof. Satoshi Watanabe (The University of Tokyo), Prof. Katsuyuki Fukutani (The University of Tokyo), Prof. Noriaki Takagi (The University of Tokyo), Prof. Junji Nakamura (Tsukuba University), Prof. Tadahiro Komeda (Tohoku University), and Dr. Ryuichi Arafune (NIMS).

Understanding the dynamics of atoms and molecules at surfaces and interfaces has been becoming increasingly important in a wide range of research fields from basic science to applied fields. Surfaces and interfaces play an important role in energy and mass transfer in materials. Application of nanotechnology in various industrial fields promotes the research for novel nanoscale and/or low dimensional materials. In addition, the recent experimental and theoretical progress such as scanning probe microscopy, synchrotron radiation and laser spectroscopy, first-principles density functional theory calculation, etc. has made it possible to elucidate and control the processes at surfaces in atomic scale.

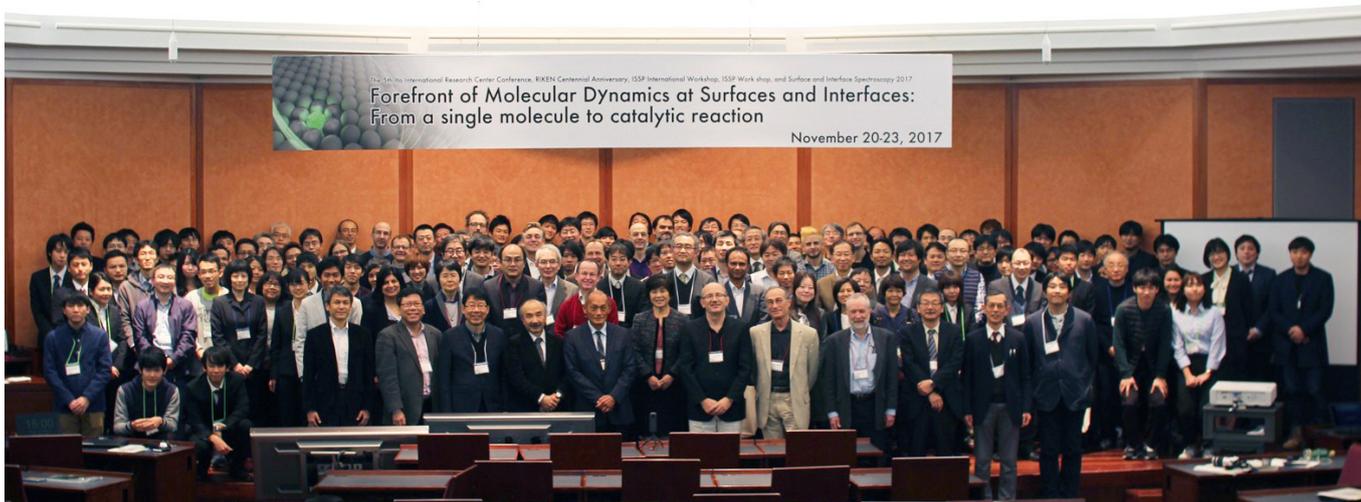
This international conference focused on molecular dynamics at surface and interface. The oral and poster presentations were performed concerning the following topics:

- Physics and chemistry of adsorbed molecules
- Low dimensional materials at surface and interface
- Dynamical processes at model catalysts
- Molecular processes at the surface and interface of devices
- Elementary processes at solid-liquid interface.

Hot discussions were held not only during the symposium but also during tea-breaks and meals. During and after the conference, we have received a lot of positive comments on the high-quality presentations and operations of the meeting. We would like to acknowledge all the participants, the committees and secretaries.

The abstract booklet of this conference can be downloaded from the following URL;

[http://yoshinobu.issp.u-tokyo.ac.jp/IIRC5\\_Program\\_booklet-Final.pdf](http://yoshinobu.issp.u-tokyo.ac.jp/IIRC5_Program_booklet-Final.pdf)



## Computational Materials Science —Now and the Future—

April 3 - 4, 2017

H. Noguchi, N. Kawashima, O. Sugino, H. Watanabe, S. Kasamatsu,  
Y. Noguchi, S. Morita, T. Ohtsuki, A. Kitao, and Y. Morikawa

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. The selected topics include the target of the post-K supercomputer project, the progress made in the elements strategy projects, the emergent data-driven material research, and “the Project for advancement of software usability in materials science” that developed the numerical library K $\omega$  to solve the shifted linear equation within the Krylov subspace and numerical solver package mVMC of the many-variable Variational Monte Carlo method in 2016. In addition to 16 invited talks and 30 poster presentations, two special lectures for machine-learning were given by Prof. Masayuki Ohzeki and Dr. Daisaku Yokoyama.



## Small Angle Neutron Scattering, Neutron Reflectivity, and Neutron High-Resolution Instruments

April 24 - 25, 2017

M. Shibayama, O. Yamamuro, and M. Hino



It has already passed more than 6 years since the shutdown of the Research Reactor, JRR-3, due to the Great Earthquake on March 11, 2011. During this period until today, demands of neutron scattering/reflectivity/spectroscopy experiments for nanometer-order structural analyses and investigations of dynamics have been increasing rapidly than before. Neutron Science Laboratory (NSL) held a workshop on instrumentations and state-of-art researches with small-angle neutron scattering, neutron reflectivity, and high energy-resolution instruments during the period of April 24 - 25, 2017. Since restart of JRR-3 was expected to be February, 2018, it was a timely project and more than 100 scientists as total participated in this workshop during the two-day workshop. On Day 1, the workshop began with an introductory remarks by Prof. Takigawa, Director of ISSP, and

Prof. Shibayama, Director of NSL, followed by presentations by instrument scientists about the current status and future plans of each instrument. After these presentations, a summary talk and free discussions were given, where importance and necessity of collaborations between JRR-3 and J-PARC MLF, not only on organization level but also from educational viewpoints, was emphasized. Then, a mixer was held in the lounge. On Day 2, scientific highlights from various fields were given, such as polymers, composites, proteins, liquid structures, multi-ferroic solid materials, and structure transitions in liquids. In general discussions and summary session, there were a few remarks were addressed: (1) importance of diversity of soft matter science, but the necessity of viewpoints with universality, (2) how to improve the general-use program of neutron scattering, (3) how to increase the number of neutron users, (4) safety and security issue. It was a very successful workshop from various viewpoints, science, instrumentation, and general-use program. The workshop was closed by looking forward to restart of JRR-3.



# Frontier Science of Electronic Properties Observed/Manipulated by Light: Strong Correlation, Topology, Low Dimension and Dynamics

June 12 - 14, 2017

T. Kondo, H. Wadati, H. Akiyama, and A. Kimura

The photoemission is a powerful technique to directly observe electronic structure of matter, and it has established itself as an experimental tool commonly used in the research of condensed matter physics. While this trend on photoemission will be continued in the future as well, further enhancement of capability in this technique is highly expected for younger generation. Until now, it has been well accepted that the discovery of new materials such as high temperature superconductors and topological insulators, and the following observations of superconducting gap and spin-polarized texture in these have boosted the development of photoemission technique. Together with the demand to investigate these physical properties, the photoemission has also forcefully evolved forward keeping in step with the progress of advanced light source. In recent years, synchrotron and laser, which has been being developed independently with each other, are getting overlapped in the range of photon energy. We have now entered an era in which researchers can freely select these light sources to use in a cross-sectoral manner, depending on each experimental purpose. A dream to cutting edge research on materials science with photoemission will greatly expand as long as one makes the most use of "coherence", "polarization", and "pulse", the three biggest advantages for controlled light. Based on these background, in this work shop, active young researchers have gathered in ISSP to discuss the potential and capability of photoemission and how to utilize it for the future materials science.



## Recent Progress in the Research of the 5d Pyrochlore Oxides

August 2, 2017

T. C. Kobayashi and Z. Hiroi

The workshop was planned as an opportunity for researchers working on various 5d transition metal pyrochlore oxides to get together and discuss their recent progress. The 5d pyrochlore oxides are now well recognized as interesting playgrounds for novel physics associated with spin-orbit coupling. The Weyl semimetal behavior and the all-in-all-out magnetic order are observed in  $\text{Ln}_2\text{Ir}_2\text{O}_7$  and  $\text{Cd}_2\text{Os}_2\text{O}_7$ , in which also electron correlations play an important role. The spin-orbit coupled metal  $\text{Cd}_2\text{Re}_2\text{O}_7$  is another hot topics, which may exhibit multipole orders and parity-mixing superconductivity. Other pyrochlore

oxide  $\text{CsW}_2\text{O}_6$  with the  $5d^{0.5}$  electron configuration seems to be a candidate for the molecular orbital crystal with trimerization. Approximately 40 people joined the meeting. The workshop gave a wonderful opportunity for attendees to understand the present status and to imagine the future prospect of the 5d pyrochlore oxides.



## The 9th APCTP Workshop on Multiferroics

November 9 - 11, 2017  
T. Kimura, T. Arima, and M. Tokunaga

The APCTP Workshop on Multiferroics started at the headquarter of Asia Pacific Center for Theoretical Physics (APCTP) at Pohang in 2008 and has continued as an annual event for the last several years. It has successfully brought together the most active members in the field of multiferroics and continues to enhance the strength of collaboration in the international community, particularly in APCTP member countries. In 2017, the 9th workshop was held at Kashiwa campus, University of Tokyo. We had 23 invited talks (14 from APCTP member countries and 9 from non-APCTP member countries), 6 contributed talks (4 from Japan and 2 from non-APCTP member countries), and 55 poster presentations mainly by graduate students and young researchers. During the three days, participants of the workshop actively discussed various topics related to multiferroic research such as fundamental understandings of known multiferroics, syntheses of new multiferroics, fabrications of multiferroics/ferroelectrics with new functionalities, multiferroic domain engineering, and explorations of new functionalities (e.g., electric control of magnetism and nonreciprocal phenomena) in multiferroics. Furthermore, we had a special session during the reception where all the participants frankly discussed the future direction of multiferroic research. During and after the workshop, we received a number of positive comments from the participants. Some of them mentioned that they are going to start collaboration work with other participants. Some young participants acknowledged our financial supports (or no registration fee). From these comments from participants, we consider to achieve the purpose of the workshop.



## ISSP - J-PARC Joint Workshop on Science Frontier by Neutron Scattering: The 16th Korea-Japan Meeting on Neutron Science

January 8 - 10, 2018

T. Masuda, M. Shibayama, K. Nakajima, and H. Seto

Neutron scattering research in wide field was discussed by Korean and Japanese scientists. The workshop consists of the following contents: (i) facility reports (ii) magnetism and strongly correlated electrons (iii) industrial use (iv) instruments, software, and advanced data analysis (v) Biological and soft matter and (vi) liquid. In the facility report, current status of neutron science laboratory institute for solid state physics (NSL-ISSP) was reported by the director Prof. M. Shibayama. During the long shut down of JRR-3, NSL-ISSP supports the travel budget for neutron experiments in foreign facilities for JRR-3 users. About high-resolution chopper spectrometer (HRC) cooperated by NSL-ISSP and KEK, combination of various sample environment devices, upgrade of Fermi chopper, and the increase of the beam power of J-PARC made the HRC efficient instrument, and the scientific productivity has been improved. Status of other neutron facilities were presented by the directors. Research topics including observation of magnon-phonon coupling in manganites by Je-Geun Park, Kitaev quantum spin liquid by S. Ji, and small angle neutron scattering on skyrmion by T. Nakajima were reported in the field of magnetism. Unique neutron techniques such as neutron holography for the investigation of local atomic structures by K. Ohyama were introduced. In the field of soft matter science, structure analysis of critical gelation cluster by X. Li, neutron reflectivity measurements for diffusion dynamics of polymer melts by J. Koo, and many interesting talks were presented. In total 28 of oral and 32 of poster presentations were made by Korean and Japanese scientists, and the participants had fruitful discussions.



## Status of SPring-8 BL07LSU and Strategies to Genesis of the Next-Generation Soft X-ray Science

March 13, 2018

I. Matsuda, S. Shin, F. Komori, Y. Harada, and H. Wadati

Synchrotron radiation laboratory at the Harima branch develops the frontier science at high-brilliance soft X-ray beamline BL07LSU at SPring-8 and makes the experimental innovations with domestic and foreign users. We have performed time-resolved, spatial-resolved and energy-resolved soft X-ray spectroscopy to study electronic states and their dynamics of new materials. Recently, we have also carried out *operando* experiments to examine functional materials under the working conditions. This year, we celebrate 10 years since construction of the beamline, reaching a milestone to consider the next project. On the other hand, new light sources, such as XFEL or a diffraction limited storage ring, are recently encouraged to be designed and to be constructed over the world. In Japan, we have plans of Slit-J and SPring-8-II. Since science and techniques, developed at BL07LSU, are closely related to experiments expected to be held at such new generation synchrotron radiation sources, it is also high time to consider the next soft X-ray science. Thus, we organized this ISSP workshop to present our recent achievements and to discuss the strategies with participants.

We had two invited talks by two outstanding researchers. Prof. Kotsugi prospected the future of synchrotron radiation researches and Dr. Katayama presented his recent results at SACLA. Speakers talked about their recent results from each end station (time-resolved spectroscopy, 3D nano-ESCA, emission spectroscopy, ambient pressure XPS and so on). During the discussion time, we shared information on the frontier researches of synchrotron radiation in various fields, physics, chemistry, and biology. Eventually, we were able to make the clear vision for the next-generation soft X-ray science at BL07LSU and at new storage rings. We also encouraged a young researcher by awarding the best poster prize.



