# **ISSP** Workshops

## Future Research of Material Science Using Vacuum-Ultraviolet and Soft X-ray Synchrotron Light

May 28-29, 2013 J. Fujimori, T. Kinoshita, K. Amamiya, T. Okuda, S. Shin, J. Yoshinobu, and F. Komori

Vacuum-ultraviolet and soft X-ray beamlines have been updated in the synchrotron light facilities in Japan including SPring-8 and Photon Factory. In the end stations of these beamlines, advanced techniques for the studies of new materials are now available by the improvement of polarization control and expansion of wavelength range with high energy resolution, and so on. Using these, we can expect more precise and quantitative measurements for studying new properties of the materials. However, the synchrotron radiation facilities have lacked enough opportunities to share information on their individual development plan. This is not ideal for the present trend in the research of solid state physics that a target material is intensively inves-

tigated by several complimentary methods for the thorough understanding of its properties and functionalities through cooperative research. In this workshop, there were reports on the current status and future plan of each synchrotron radiation facility in Japan and on the recent results at the advanced beamlines including some of the oversea facilities as well as on the plan of Tohoku medium-size synchrotron radiation facility. Based on these reports, we discussed the future research using vacuum-ultraviolet and soft X-ray synchrotron light. The workshop provided an important opportunity for the community of this research area that the beamline scientists from all the facilities and active users in Japan intensively discussed the future of their research field together.



#### Energent Quantum Phases in Condensed Matter (EQPCM2013)

June 12-14, 2013 Y. Takada and M. Oshikawa

This ISSP workshop was held as the symposium part of the international workshop of the same title. See the section of "International Conferences and Workshops".

#### Polar Oxides for Energy Conversion

The focus of this workshop was on new oxide materials related to energy conversion applications. In particular, new types of polar oxides may offer a way to design internal electric field gradients in oxide heterostructures for achieving efficient photo-

carrier separation. In addition to basic solar cell geometries, the desire is to use functional oxides that fulfill two roles simultaneously, harvesting solar light by photocarrier generation and catalytically enhancing photoelectrochemical reactions on the surface. The presentations covered a broad range of related topics: catalytic materials, synthesis techniques, surface analysis, crystal design, phase transition mechanisms, and microstructural analysis. About 40 people attended the workshop, most of whom are young researchers. The event was thus a good venue for in-depth discussions on new materials and new ideas on oxide materials design. Two longer invited talks gave the attendees a chance to think about more general materials lifecycle issues and to see a practical example how new materials, in this case thermoelastic alloys, transition from pure basic science research to an actual application.



#### Extreme High Magnetic Field Science: Towards Fusion of Field, Materials and Probe

October 30-November 1, 2013 K. Kindo, H. Ota, T. Sasaki, T. Shimizu, S. Takeyama, M. Tokunaga, H. Nojiri, M. Hagiwara, Y. Hosokoshi, Y. H. Matsuda, M. Yoshizawa, and S. Mitsudo

Recently, large high-magnetic field laboratories have been built in many countries all over the world. Progress in the last decade on both generation- and measurement-techniques makes it possible to carry out various experiments under high magnetic fields. New development of materials science has started, as well, such as a fusion of high field with other fields (*e.g.* synchrotron radiation light source or laser). A fusion of high magnetic field, new materials and probe is required to develop

an advanced research on materials science for the next decade. High Magnetic Field Co-laboratory Project also contributes to the progress of high field science. The project was planned to connect Japanese large high field laboratories strongly and has been realized partially. An exchange of researcher has been promoted in accordance with the project. This workshop was held to discuss the issues noted below.

- 1) Search for a new research subject for the next decade and training
- of young researchers
- 2) Development of research subject fused with other fields

3) Complete realization of High Magnetic Field Co-laboratory Project The three issues were discussed not only by the high field laboratories but also by the users community. It was very significant for the high field community that all researchers concerned with high field gathered together to discuss the above issues and exchange recent information.





June 26, 2013 M. Lippmaa, Y. Matsumoto, and I. Takeuchi

### Materials and Physical Sciences Related to Energy and Environment

November 11-13, 2013

H. Mori, K. Kanoda, T. Sasaki, J. Takeya, F. Komori, M. Shibayama, J. Yoshinobu, O. Yamamuro, H. Akiyama, O. Sugino, Y. Harada, and M. Lippmaa

After the 2011 Tohoku earthquake, the scientific studies towards energy conversion and green environment have been extensively carried out. This workshop has focused on fundamental researches of novel materials and physical sciences related to energy and environment.

The energy conversion system and recent novel materials have hierarchical structures. For example, solar cell is a complex system, composed of synthetic molecules, charge transfer pairs, p-n interface, semiconducting layers, and buttery device. As attractive soft material, ionic liquid is also a hierarchical system with nano-meso-micro correlation lengths. The scientific



In this workshop, the active 39 researchers have afforded 30-min. keynotes and 20-min. oral presentations in the sessions of "solar cell artificial photosynthesis", "photo-catalyst", "battery", "surface science", "molecular materials organic electronics", "bio-materials", and "hydrogen-based-materials". The 24 graduate students and young researchers have presented their researches in the poster session. Totally, 198 participants for 3 days participated in the workshop with hot discussions. It is meaningful that prominent researchers in a wide range of scientific fields presented their cutting-edge research results and exchange their information.



### Condensed Matter Physics under Pulsed Ultrahigh Pressures and Magnetic Fields

November 25-26, 2013 K. G. Nakamura, T. Suemoto, N. Sarukura, S. Koshihara, H. Noziri, and M. Yoshimura

Ultrahigh pressures (>1TPa) and magnetic fields (>1kT) are recently realized by using a high-power laser, and electronic and structure dynamics in condensed matter can be studied under these extreme conditions. In this symposium, we discussed generation techniques of such extreme fields, current research activities, and future topics. The symposium consisted of sessions on (1) physics under strong magnetic fields, (2) physics under ultrahigh pressures, and (3) ultrafast measurements, with seventeen presentations. On the topics (1) there were presentations of a recent generation technique of the kT magnetic field using high-power laser plasma and measurements with synchrotron radiation, laser, and neutron diffraction under pulsed magnetic fields. On the topics (2), the generation of laser-induced ultrahigh pressures over TPa, which cannot be accessed by

static compression, and combination research works with X rays from XFEL (X-ray Free Electron Laser) were presented. In addition, studies on planetary science using shock-induced high pressures were also presented. On the topics (3), single-shot measurement techniques are presented to study ultrafast phenomena using laser combined with pulsed electrons and X rays. Throughout the symposium, we discussed the problems of pulsed high pressure and magnetic fields and potential for studying unique properties of materials under non-equilibrium conditions.



#### Local Symmetry Breaking and Quantum Properties in Strongly Correlated Electron Systems

November 27-29, 2013 T. Arima, H. Harima, S. Nakatsuji, and Z. Hiroi

Symmetry is one of the most important concepts to determine the physical properties of solid states. For example, many interesting phenomena such as unconventional superconductivity, multiferroicity, and spin Hall effect are relevant to the breaking of the global space-inversion symmetry and resultant antisymmetric spin-orbit interaction. The antisymmetric spin-orbit interaction can be activated at non-centrosymmetric atomic sites even in materials with global space inversion symmetry. At such non-centrosymmetric sites, an odd-parity ligand field also allows the emergence of odd-parity multipoles like magnetic quadrupole and electric octupole moments, which may open the door to new paradigms in material science.

This workshop was organized to shed light on the possible exotic properties induced by the breaking of local inversion symmetry coupled with the electron correlation and spin-orbit coupling. During the workshop, off-diagonal responses,

quantum transport, and exotic superconductivity were intensively discussed in terms of multipoles. In particular, many itinerant systems hosting the degree-of-freedom of various multipole moments were intensively discussed. The number of participants reached 87, consisting of researchers in the fields of 4f-electron systems (rare-earth compounds), 5f systems (uranium compounds), and d-electron systems (transition-metal compounds). The discussions across the various communities in solid state science made the workshop very successful.



#### Joint Research Meeting of ISSP Supercomputer Joint Use and CMSI Annual Activity Report 2013

December 10-13, 2013

H. Akai, N. Kawashima, O. Sugino, S. Todo, H. Noguchi, T. Oguchi, A. Oshiyama, T. Kawakatsu, S. Tsuneyuki, N. Hatano, S. Kasamatsu, H. Watanabe, Y. Noguchi, H. Shiba, and S. Morita

Every year, we hold a workshop for the joint research of the ISSP supercomputers. This year, the meeting was co-organized with The Computational Materials Science Initiative (CMSI), of which ISSP is the headquarters. During the four days of the meeting, we had 58 oral presentations, and 49 poster presentations. 192 scientists participated. The subjects of the presentations ranged from the most fundamental low-temperature behaviors of quantum matters to semi-conductor device, and new energy resources. We invited five distinguished speakers: K. Nakajima (U. Tokyo), Z. Hiroi (ISSP), K. Hukushima (U. Tokyo), M. Kato (Tokyo Inst. Tech.) and Y. Oyanagi (Kobe Univ.). We had active discussions for oral and poster presentations. The results of questionnaire on ISSP supercomputer were also presented and supercomputer architectures suitable to computational material science were discussed. The following three people are presented awards.

Young Researcher Encouragement Award: Kazuya Ishimura (Institute for Molecular Science).

Visual Award: Takuma Yagasaki (Okayama University).

Poster Award: Hiroshi Watanabe (Institute for Solid State Physics).





#### Joint Researches in Foreign Neutron Facilities

#### January 29-30, 2014 T. Masuda, M. Shibayama, H. Yoshizawa, and O. Yamamuro

Since the Great East Japan Earthquake on 11th March in 2011, Japan Research Reactor (JRR3) has suspended its operation and the Neutron Scattering Laboratory (NSL) has had difficulty in the domestic joint research using neutron spectrometers installed in JRR3. Now the NSL provides the neutron users the travel budgets for the neutron experiments at foreign facilities and supports the joint researches. In this workshop the users presented and discussed the researches performed at the foreign facilities. The field covers wide range including magnetism, strongly correlated electrons, glass, and soft matter. As for magnetism, the topics on geometrically frustrated systems were focused; the complex magnetic structure in chiral magnet, novel magnetic phase in quantum spin ice, the interplay between magnetic structure and electric polarization in multiferroics, etc. As for strongly correlated electrons system, studies on magnetic excitations and structures in various types of superconductors



including high- $T_c$  Cu oxides, Fe pnictides, and heavy-fermion materials were presented. It should be noted that the development and application of high pressure cell were implemented even in the restricted machine time at foreign facilities. Structural and dynamical analyses on new materials in the field of soft matter and quasi-elastic scatterings on cluster structure and ion liquid in the field of glass were reported. With 25 talks and 17 posters, the discussions at the workshop were hot and fruitful, indicating the scientists in the field of neutron scattering are actively doing their research and even enjoying this hard situation.

#### Present Activity and Future Prospect of BL07LSU in SPring-8

February 19, 2014 S. Shin, F. Komori, I. Matsuda, and Y. Harada

Five years has passed since the University of Tokyo started constructing an undulator beamline BL07LSU in SPring-8, and it is the middle of the project period using exclusively the beamline for joint studies. Polarization-controlled high-brilliance light is now available in the beamline, and used for advanced spectroscopy at the end-stations for material science. The number of publications from the beamline users has increased recently, and attracted much attention over the world. As a result, the overseas researchers continuously apply their joint studies there, and more than 30 % of the beam time for the joint studies is used with the foreign collaborators at present. In this workshop, the present status of the undulator light and the recent results at the end-stations were reported, and the advancement of the beamline in the next five years was discussed. In particular, future use of the polarization switching was proposed in relation to the development of the variable-polarization undulator. For the next two years, three long-term projects have been accepted at the three stationary end-stations for time-resolved spectroscopy, three-dimensional nano ESCA and soft X-ray emission spectroscopy. Each research plan with common keywords of operando

and polarization control was introduced and discussed. New research plans using the free port were presented as well.

