STXM Users Meeting

Date: June 4, 2012
Place: Conference Room C, Okazaki Conference Center, Okazaki, Japan

June 4th (Mon)

<Session 1: Reports of UVSOR Facility, Chair: A. Ito>

13:30-13:35 M. Katoh (UVSOR)
Introduction from director

13:35-13:50 T. Ohigashi
Current status of BL4U beamline

13:50-14:00 H. Arai (UVSOR)
Introduction of STXMs of oversea synchrotron radiation facilities

14:00-14:10 M. Adachi (IMS)
Current status of UVSOR-III

14:10-14:20 N. Kosugi (IMS)
Collaboration programs of IMS

14:20-14:45 Coffee Break

<Session 2, Chair: T. Ohigashi>

14:45-15:00 A. Ito (Tokai Univ.)
Soft X-ray spectro-microscopy of biological samples

15:00-15:15 T. Araki (TOYOTA Central R&D Lab.)
(Untitiled)

15:15-15:30 H. Yabuta (Osaka Univ.)
Innovative researches by STXM; outer space, the earth and life

15:30-15:45 J. Usukura (Nagoya Univ.)
Spatial structure of actin cytoskeletons revealed by various imaging methods

15:45-16:00 N. Iwata (Ricoh)
Imaging of organic materials by using STXM

16:00-16:15 Y. Ishii (Nagoya Institute Tech.)
Development of functional materials based on nano-carbon

16:15-16:30 A. Matsuura (Fujita Health Univ.)
Early diagnosis of pediatric patients with Wilson disease by synchrotron copper imaging

16:30-16:45 K. Shinohara (Waseda Univ.)
Observation of living cells by a contact microscope with laser-produced plasma X-rays

16:45-17:00 Coffee Break

<Session 3, Chair: T. Araki>

17:00-17:15 K. Ono (KEK)
Observation of the magnetic domains of NdFeB magnet

17:15-17:30 Y. Takeichi (KEK)
Summary of the STXM project at PF

17:30-17:45 N. Inami (KEK)
Development of the real-time control and the measurement system for the STXM

17:45-18:00 Y. Yamamoto (Nagoya Institute Tech.)
Action mechanism of anesthetic molecules by interfacial chemical approach

18:00-18:15 T. Tominaga (JSR)
Structural analysis of JSR polymer materials by using synchrotron radiations

18:15-18:30 H. Kihara (Ritsumeikan Univ.)
Current status of the full-field imaging microscope at Ritsumeikan Univ. and expectation for new STXM

18:30-18:45 R. Mizutani (Tokai Univ.)
Three-dimensional structural analysis of brain tissue by microtomography

18:45-19:30	T. Ohigashi (UVSOR)
	Discussions
19:40-21:00	Banquet

UVSOR Workshop on Novel Development for Low-Energy Photoemission Spectroscopy at UVSOR-III

Date: June 21-22, 2012
Place: Seminar room (#201) of main building, Institute for Molecular Science, Okazaki, Japan

June 21th (Thu)

13:00-13:30 Registration

<Session 1, Chair: K. Soda>

13:30-13:40 M. Matsunami (UVSOR)
Opening remarks

13:40-14:00 M. Adachi (UVSOR)
Present status of UVSOR-III

14:00-14:25 K. Tsuchiya (KEK-PF)
Design of variably polarized undulator

14:25-14:45 T. Ito (Nagoya Univ.)
3D-ARPES for strongly correlated quasi-2D system $GdTe_2$

14:45-15:05 H. Miyazaki (Nagoya Institute Tech.)
Electronic structure of rare-earth oxide thin films studied by 3D-ARPES

15:05-15:30 T. Hirahara (Univ. Tokyo)
Spin-polarized surface electronic states of non-magnetic ultrathin films

15:30-15:55 T. Ujihara (Nagoya Univ.)
Effect of minibands and periodic modulations in semiconductor superlattice structures

15:55-16:25 Coffee break

<Session 2, Chair: M. Matsunami>

16:25-16:50 S. Tanaka (Osaka Univ.)
Low-energy ARPES of HOPG

16:50-17:15 T. Takeuchi (Nagoya Univ.)
High-resolution photoemission spectroscopy for thermoelectric-material development

17:15-17:40 K. Ishizaka (Univ. Tokyo)
Spin-orbit interaction studied by low-energy ARPES

17:40-18:05 R. Yoshida (ISSP)
Hidden-order transition in URu_2Si_2 studied by ultrahigh-resolution ARPES

18:05-18:30 K. Shimada (HiSOR)
Development and perspective for precise analyses of the electronic structure in solids by low-energy synchrotron radiation ARPES

18:30-19:00 Facility tour

19:00-21:00 Banquet

June 22th (Fri)

<Session 3, Chair: S. Kimura>

09:00-09:30 G. Zhang (NSRL)
Introduction of the ARPES facility and the upgrade program of Hefei Light Source

09:30-09:50 H. J. Im (Hirosaki Univ.)
Low-energy excitation in A-site ordered perovskite $CaCu_3Ti_4O_{12}$ studied by hν-dependent ARPES

09:50-10:15 K. Nakayama (Tohoku Univ.)
High-resolution ARPES study of superconducting gap symmetry in Fe-based superconductors

10:15-10:40 S. Kera (Chiba Univ.)
Photoemission spectroscopy for organic semiconductor films: electron-phonon coupling and band gap states

10:40-11:10 Coffee break

<Session 4, Chair: T. Ito>
11:10-11:35 H. Kumigashira (KEK-PF)
In-situ synchrotron-radiation photoemission study for surface and interface in strongly correlated oxide heterostructures
11:35-12:00 M. Fujisawa (ISSP)
Design of low-photon energy VLS-PGM of BL5U
12:00-12:20 S. Kimura (UVSOR)
Discussion
12:20-12:30 **Closing remarks**

UVSOR workshop “Perspectives of the beamline for organic solids at UVSOR”

Date: Sep 25-26, 2012
Place: Seminar room (#304) of UVSOR building, Institute for Molecular Science, Okazaki, Japan

Sep 25th (Tue)

13:30-13:40 **Opening Remarks**

<Session 1, Chair: S. Kera>

13:40-14:05 M. Adachi (UVSOR)
Present status of UVSOR-III

14:05-14:35 H. Ishii (Chiba Univ.)
Research of interfacial electronic structures of organic semiconductors by electron spectroscopy

14:35-15:00 Y. Nakayama (Chiba Univ.)
Valence band structure of organic single crystals challenged by synchrotron radiation photoelectron spectroscopy

15:00-15:25 S. Tanaka (Shimane Univ.)
Photoelectron spectroscopy of organic thin films under light irradiation

15:25-15:55 Coffee break

<Session 2, Chair: K. K. Okudaira>

15:55-16:20 I. Yamamoto (Saga Univ.)
Researches on electronic structure of organic thin films at Saga University beamline BL13 in SAGA-LS

16:20-16:50 T. Hosokai (Iwate Univ.)
A systematic study of correlation between org/metal interface electronic structure and bonding distance by using X-ray standing waves technique and angle resolved photoemission spectroscopy

16:50-17:20 H. Yoshida (Kyoto Univ., PRESTO)
Depth resolved electronic structure of organic solids with angle resolved X-ray photoemission spectroscopy and multivariate analysis

17:20-17:50 T. Sakurai (Univ. of Tsukuba, PRESTO)
Investigation of properties at electrode interfaces in organic solar cells using synchrotron-based analytical techniques

17:50-18:30 Break

18:30- Banquet

Sep 26th (Wed)

<Session 3, Chair: H. Ishii>

9:00-9:30 D. Yoshimura (SAGA Light Source)
Memories of UVSOR BL8B2 and outline of the soft X-ray beamlines at SAGA-LS

9:30-10:00 K. Mase (Photon Factory)
Present status and prospects of a high-brilliance VUV/SX beamline BL-13A in PF; expectations for the beamline dedicated for organic solids in UVSOR

10:00-10:30 H. Yamane (UVSOR)
Present status of high-resolution ARPES system at BL6U for various solids and surfaces

10:30-11:00 T. Ito (Nagoya Univ.)
VUV Angle-Resolved Photoemission Study of Quasi-One-Dimensional Organic Conductors

11:00-11:25 K. Shimada (HiSOR)
Studies of surface electronic structures of organic materials at HiSOR

11:25-13:00 Lunch Break

<Session 4, Chair: S. Tanaka>

13:00-13:30 K. Kanai (Tokyo Univ. of Science)
Electronic structure of various organic materials probed by synchrotron radiation

13:30-14:00 T. Miyazaki (Ehime Univ.)
Photoelectron Spectroscopy of Endohedral Metallofullerenes

14:00-14:25 K. Okudaira (Chiba Univ.)
Evaluation of molecular orientation by ARUPS

14:25-14:55 S. Kera (Chiba Univ.)
Photoelectron angular distribution from valence band of organic thin films: Reconstruction view of molecular orbitals

14:55-15:20 Discussion: Perspectives at BL2B

15:20- **Closing Remarks**

UVSOR Symposium 2012

Date: Nov 10-11, 2012
Place: Okazaki Conference Center, Okazaki, Japan

Nov 10th (Sat)

<Session 1, Chair: M. Katoh>

13:00-13:15 M. Katoh (UVSOR)
Opening remarks

13:15-13:30 N. Kosugi (IMS)
Evaluation of UVSOR and perspective of IMS

13:30-13:50 M. Adachi (UVSOR)
Present status of UVSOR-III

13:50-14:20 T. Ohigashi (UVSOR)
Perspective for applicative observations by using a scanning transmission X-ray microscopy

14:20-14:40 A. Ito (Tokai Univ.)
Biomedical application of soft X-ray scanning microscope

14:40-15:00 Coffee Break

<Session 2, Chair: M. Matsunami>

15:00-15:20 T. Hirahara (Univ. Tokyo)
Electronic structure of ultrathin Bi films: influence of the substrate and its implication on topological properties

15:20-15:40 T. Hajiri (Nagoya Univ.)
Polarization-dependent angle-resolved photoemission spectroscopy on LiFeAs

15:40-16:00 S. Tanaka (Osaka Univ.)
Direct observation of the electron-phonon scattering by using angle-resolved photoelectron spectroscopy

16:00-16:20 S. Kera (Chiba Univ.)
Origin of interface state for □-conjugated molecules adsorbed on metal

16:20-16:40 Coffee Break

<Session 3, Chair: E. Shigemasa>

16:40-17:00 Y. Takagi (IMS)
The X-ray magnetic circular dichroism measurement at BL4B

17:00-17:20 M. Nagasaka (IMS)
Local structures of methanol-water binary liquid studied by soft X-ray absorption spectroscopy

17:20-17:40 H. Iwayama (UVSOR)
Dissociation pathways of inner-shell ionized $C_4H_5F_3O_2$ molecules studied by an auger-electron-ion coincidence method

<Poster Session and Banquet, 18:00-21:00>

P01 K. Eguchi (IMS)
XAS/XMCD measurement of vanadyl pthalocyanine films on Si(111)

P02 T. Tajiri (Hyogo Univ.)
Development of novel nozzle for molecule spectroscopy by ultrasonic atomization method

P03 K. Soda (Nagoya Univ.)
Electronic structure of pyrite-type $Ni_{1-x}Cu_xS_2$ (I): CuS_2

P04 Y. Liu (Chiba Univ.)
Angle-resolved ultraviolet photoelectron spectroscopy investigation of transition-metal phthalocyanines thin films on graphite

P05 M. Sawa (Niigata Univ.)
Development of a high-resolution magnetic bottle electron spectrometer

P06 Y. Konosu (Niigata Univ.)
Multi-electron spectroscopy of condensed water molecules

P07 H. Zen (Kyoto Univ.)
Intense and short pulse generation by CHG-FEL utilizing pulse compression

P08 Y. Inaguma (Gakushuin Univ.)
Photoluminescence upon vacuum ultraviolet excitation in $M_3(PO_4)_2$:Pr^{3+} (M = Ca, Sr, and Ba)

P09 Y. Uematsu (Nagoya Univ.)
Performance of new optical klystron at UVSOR and application to CHG

P10 Y. Hida (Nagoya Univ.)
Study of pulsed sextupole magnet system for beam injection at UVSOR

P11 M. Sato (Tohoku Univ.)
Local structure analysis of zeolite synthesized from blast furnace slag

P12 Y. Nakamura (Fukui Univ.)
Development of spectroscopic ellipsometry for UV-VUV region

P13 T. Toyoda (Fukui Univ.)
A Study of visible photoluminescence in boron-doped diamond thin films

P14 D. Itoh (Fukui Univ.)
Band structure of CN_x

P15 K. Fujita (Fukui Univ.)
Ultra-violet photoluminescence spectra from AlGdN by core excitation

P16 K. Hayashi (Gifu Univ.)
Characterization of photoinduced phenomena in amorphous chalcogenide semiconductors

P17 T. Niwa (Nagoya Univ.)
Development of an electron beam bunch length measurement system for the transmission-type polarized electron source

P18 M. Kaneko (Nagoya Univ.)
Angle-resolved photoemission spectroscopy of $Sm_{1-x}Y_xS$

P19 Y. Inaba (Waseda Univ.)
XANES analysis of electronic structure of Mn in $La_{1-x}A_xMnO3\pm\square$ (A=Ca, Ba)

P20 Y. Shingaki (Waseda Univ.)
Local environment analysis of dilute rare earth elements in phosphor materials

P21 H. Miyazaki (Nagoya Institute Tech.)
Electronic structure of half-Heusler type ZrNiSn alloy

P22 H. Miyazaki (Nagoya Institute Tech.)
Electronic structure of K-doped EuO ultrathin films

P23 K. Yoshida (Kyoto Univ.)
Analysis of the electric status of ZnO treated by microwave

P24 S. Kimura (UVSOR)
IR micro-spectroscopic imaging using SR from UVSOR-III

P25 H. Katayanagi (IMS)
Photodissociation dynamics of fullerenes by velocity map imaging with improved mass resolution

P26 Y. Takagi (IMS)
Magnetic property of iron phthalocyanine on the metallic substrates

P27 H. Yamane (IMS)
Weak intermolecular interaction of organic crystalline films revealed by high-precision valence-band dispersion measurement

P28 H. Arai (UVSOR)
Development to solutions in the scanning transmission soft X-ray microscopy at BL4U of UVSOR

P29 T. Shimada (Nagoya Univ.)
High-resolution angle resolved photoemission spectroscopy of $FeSb_2$

P30 Y. Imoto (Fukui Univ.)
Current status of the VUV beamline BL3B (HOTRLU)

Nov 11th (Sun)

<Session 3, Chair: S. Kimura>
9:00-9:30 M. Kitaura (Yamagata Univ.)

Formation and relaxation of photo-excited states of localized electron systems induced by excitation with vacuum ultraviolet photons

9:30-9:50 T. Nakazato (Osaka Univ.)
Temperature dependence of rare-earth doped APLF glass photoluminescence

9:50-10:10 R. Ishikawa (NAOJ)
Development of chromospheric Lyman-alpha spectro-polarimeter (CLASP) with BL7B

10:10-10:30 K. Fukui (Fukui Univ.)
Current status of the VUV beamline BL3B (HOTRLU)

10:30-10:50 K. Nakagawa (Kobe Univ.)
Toward a complete measurement of wide-range-absorption spectra of 20 protein amino acids, 5 nuclear bases and 3 dipeptides

10:50-11:20 Coffee Break

<Session 5, Chair: T. Ito>

11:20-11:50 M. Kamada (Saga Univ.)
Personal review of UVSOR-I generation

11:50- K. Soda (Nagoya Univ.)
Discussion and closing remarks

Appendix

Review of Beamlines and Science at UVSOR

1. Overview

I was asked by the Director General to review the present status and future directions of science using UVSOR from the perspectives of

- international activities
- application to molecular science
- in-house contributions and challenges in the area of molecular science

My comments are based on the recent (2010, 2011) annual reports and a series of nine one-hour sessions with UVSOR researchers and UVSOR users from other departments in IMS and other institutions. I thank all the presenters for the careful work they put into their presentations, which allowed me considerable insight into the present status and future directions. I was particularly struck by the relative youth and enthusiasm of many of the presenters which speaks well for the vitality of UVSOR and IMS.

Here I make selected comments on each presentation / area of research / status of the instrumentation. After that I make some general observations on how these current activities position UVSOR relative to other facilities with strong research programs in molecular science, and where I think there are opportunities for improving international participation and enhancing the relevance of UVSOR research to the overall mission of IMS, which I take to be primarily fundamental research into systems and phenomena where the perspective of the molecular unit is a strong organizing principle.

2. Comments on researches

2.1 Facility and light source research (Masahiro KATOH, Director, UVSOR)

The synchrotron source, after updating to UVSOR-III in early 2012 (this year!), is a very competitive facility relative to all other sub-1GeV SR sources. The most recent upgrade has significantly reduced the emittance and has freed up space for additional insertion devices (total 6). This has provided an opportunity for adding a new, very competitive beamline for science (BL4U, STXM), a number of other beamline and end-station upgrades, and conversion of BL1U into a very versatile platform for advanced light source generation experimentation. The latter is an important aspect of a synchrotron facility as it provides ongoing challenges for the accelerator group, opportunities for collaboration with other accelerator light source facilities, and can lead to large improvements in light source technology, which may be a platform for a future upgrade of UVSOR. At the same time there appear to be too many challenging initiatives under way – free electron laser development, coherent THz systems, fs slicing, and laser Compton gamma ray generation. It was not clear which of these had priority or which had a potential or actual user community. The latter should be an important principle in guiding priorities for further investment and development in this area.

It was noted that some beamlines have challenges with operation in the current top-up mode. The fraction of the time devoted to top-up injection, and thus perturbation of the storage ring is 20% (12 seconds each minute), due to rather short lifetime of the electron beam just after the upgrade to UVSOR-III. The present 12 seconds (12 injections) per minute seem long relative to those at other SR facilities. The number of top-up injections will decrease as the electron beam lifetime and the injection efficiency improve as in UVSOR-II. Efforts should be made to improve the top-up injection procedure, as soon as possible, not only to reduce the fraction of the time, but also to reduce any perturbations of the beam position or size associated with the top-up. This is particularly important for brightness dependent experiments such as STXM.

2.2 Spectroscopy of liquid systems (BL3U: Masanari NAGASAKA, KOSUGI Group, IMS)

The liquid spectroscopy instrumentation developed at UVSOR is better than versions I have seen at the ALS and CLS. This is a very rapidly developing area of SR science with tremendous potential for both fundamental and applied studies. The cluster apparatus on BL3U is also an outstanding piece of equipment. Together with the gas, liquid and solid spectroscopy capabilities at BL3U and other UVSOR beamlines, the ensemble is ideally suited for systematic studies of the evolution of structure (electronic, magnetic and geometric) from isolated molecules/atoms, to the solid state. The session on cluster and liquid spectroscopy at the recent ICESS-12 meeting (St. Malo, France, Sep 2012) was one of the best of that conference in my opinion.

The plans that Nagasaka outlined to extend the methods to *in situ* electrochemistry, liquid-solid interfaces; solid-gas interface and *in situ* chemical and photochemical reactions are very exciting and will be some of the outstanding research from UVSOR in the next few years. This area should be supported fully. There is also very strong synergy between these spectroscopy studies and science with similar goals but with lateral spatial resolution, that will be performed on the BL4U STXM, which should

be operational and open to various classes of users by spring 2013.

2.3 VUV, EUV and X-ray absorption and photoemission spectroscopy of solids and gases (BL2A, BL4B, BL5B, BL6U: Eiji SHIGEMASA, UVSOR)

BL2A (double crystal monochromator) provides the highest energy photons at UVSOR. Despite being non-competitive relative to similar BL at other SR facilities, due to the low critical energy at UVSOR, it operates well and has a small but steady use by a number of Japanese research groups, primarily for materials science using X-ray absorption. It was noted that the publication rate was low which may reflect the non-competitive nature of this beamline. For a low energy ring like UVSOR a better choice to cover the high energy range would be a grating monochromator, which, with suitable multilayer mirror technology, can provide quite high performance up to 3 - 4 keV.

BL5B features an unusually wide photon energy range (6-600 eV) and a very large chamber equipped with a very flexible 6-axis goniometer. It is apparently one of only a few beamlines in Japan that are capable of characterizing large optical elements in a very flexible way. The research carried out on this beamline is primarily of a service character. At other facilities (e.g. ALS BL 6.3.2), there are active research programs in developing coatings and characterizing optics for semiconductor EUV lithography. This could be an area for future research at BL5B.

BL4B, the first soft X-ray beamline at UVSOR with high energy resolution, has produced some high quality molecular and materials science in recent years, based on research by in-house and external users. The newer BL3U undulator line covers a similar energy range and is now the preferred beamline for spectroscopy research in this energy range. However BL4B still has an active research program in magnetic materials (see discussion of the presentation by T. Yokoyama in section 2.7).

BL6U is the most modern and competitive of the beamlines supervised by Shigemasa. Its variable angle, variable line spacing PGM monochromator provides good intensity with outstanding energy resolution. It was noted that the minimum undulator gap that can be achieved at present is 13 mm, whereas the design specified a 10 mm minimum gap. The reason for this should be identified and repaired if possible, since there are some photon energies that cannot be reached due to the out-of-spec minimum gap. The two end stations for BL6U are each internationally competitive. The gas phase Auger electron photoion coincidence (AEPICO) apparatus is ideally suited for studies of molecular photoionization dynamics with high energy electrons, and complements research at other facilities which use the Cold Target Recoil Ion Momentum Spectrometer (ColTRIMS) approach. The MBS-A1 photoemission end station is also very competitive internationally and has been adapted for two-dimensional electron spectroscopic studies in gas phase. Consistent with its competitive character, there are a number of outstanding international collaborators (Lablanquie, Simon, Piancastelli) using this instrument.

The gas phase examples presented by Shigemasa, along with those in the 2011 UVSOR annual report are excellent examples of modern synchrotron based molecular dynamics and photo-physics science. I particularly admired the studies of ultrafast dissociation in C 1s excited CF_4 (p 53) and the electronic Doppler result in S 2p excited OCS (p 56). BL6U is one of the outstanding examples of molecular science research at UVSOR and should continue to be well supported. Identification of suitable collaborators and independent researchers from the international community should be a target for increasing the international visibility of the molecular science program at UVSOR.

I note that Shigemasa and his group members are now using the SACLA X-ray free electron laser for advanced molecular photophysics studies. This is a very good development for UVSOR. Opportunities of using research at UVSOR to complement SACLA research, possibly resulting in joint publications, should be encouraged.

2.4 X-ray absorption, X-ray emission and angle resolved photoemission of solids (BL3U, BL6U: Hiroyuki YAMANE, KOSUGI Group, IMS)

BL3U is a world class facility for X-ray absorption, X-ray emission and resonant X-ray scattering. This has enabled some exceptional research by UVSOR and outside researchers. The examples of XAS characterization of organic conductors and semiconductors for organic LED, organic electronics, and organic photovoltaic systems were fascinating. I draw particular attention to *in operando* measurements which used the difference of FY_NEXAFS spectra induced by applied potentials or currents to characterize the changes in molecular structure of electronic states (PRL 107 (2011) 147401). This is one of the first *in operando* soft X-ray studies of a device material to my knowledge. It revealed the surprising result that the electronic structure changes are associated with σ states, rather than the π states normally believed to be involved in the conductivity of organic conductors and semiconductors. These results have important implications for the field of single molecule electronic devices, which is a very hot topic and target of development at many research facilities around the world.

The X-ray emission spectrometer has exceptional performance relative to similar facilities at other SR centers. The energy resolution is below 100 meV at 140 eV X-ray energy, which is very competitive. The efficiency of the novel transmission grating spectrometer is probably the highest in the world for soft X-ray spectrometers. It has been used for studies of a number of interesting systems, including

DNA polymers (poly(G-C), poly(A-T)) and N-doped graphene nano flakes (J. Phys. Chem. C 116 (2012) 16251). The higher performance transmission grating which is planned for the XES spectrometer will further improve energy resolution and possibly efficiency. The future plan to apply XES and RIXS techniques to *in operando* studies of molecular devices is really at the cutting edge of international SR science with X-ray emission spectroscopy.

An outstanding program of angle-resolved photoemission from molecular solids and thin films on **BL6U** was also described by Dr. Yamane. The system for these studies is one of the best in the world, achieving < 5 meV overall energy resolution (photon & electron), ability to cool to 13 K, and a 5-axis motion system that allows rather complete band structure studies with the sensitivity needed to track band dispersion in organic systems which are typically much smaller than the dispersion in semiconductor and metal systems. The achievement of these technical capabilities in an instrument constructed at IMS is a tribute to the excellence of the Equipment Development Center which is a real asset for UVSOR and IMS. The quality of the preparation chamber and its ability to allow for preparation of organic thin films in a system also used for semiconductor and other samples was noted. There is strong international participation on BL6U. A number of interesting examples were outlined, including: band alignment at the interface between carbon nanotubes (CNT) and a SiC substrate in CNT rafts prepared surface decomposition of SiC (Maruyama); spin-orbit (Rashba) band splitting in 1-d Pt nanowires (Yeom); nanoscale phase separation in DNA Watson-Crick (G-C) multilayer films (Friedlein); and valence band dispersion in metal phthalocyanines (Yamane). The latter project, a major effort by Dr. Yamane, showed very fascinating temperature dependent dynamics results which gave important insights into intermolecular interactions and how these can be tuned by adding substituents to the phthalocyanine or changing the metal. Since the molecular films which are the focus of these studies are easily damaged by synchrotron radiation, it is essential to be able to prepare very uniform samples which can then be used to circumvent radiation damage by scanning the sample to fresh areas during the measurements. This system is one of the best in the world for ARPES studies of organic solids.

Dr. Yamane identified a number of improvements that could be made to further enhance the performance of this facility. These include a larger analyzer (e.g. D80 VG Scienta) to improve efficiency; a new analysis chamber; and addition of an O_2 dosing system to remove carbon contamination on the BL6U optics. To the extent these will facilitate new molecular science, UVSOR / IMS should seriously consider these requests.

2.5 Scanning Transmission X-ray Microscopy (BL4U: Takuji, OHIGASHI, UVSOR)

BL4U is a new soft X-ray undulator beamline with a dedicated STXM end station. STXM is a relatively new spectromicroscopy technique which has may applications in both fundamental and applied science. The planned science program is very ambitious. Further development of the instrumentation and techniques (cryo spectromicroscopy, cryo-tomography, ptychography) will require substantial effort, and should be staged after reliable basic operation is achieved. The STXM project at UVSOR will have a significant advantage relative to other STXM facilities, as IMS is able to provide on site sample preparation (ultramicrotomy, focused ion beam milling, high end optical microscope with encoders and micromanipulators, etc). BL4U & the STXM end station are part of the Nanotechnology Platform Project in Japan. This is very appropriate and will link the STXM to the on site analytical transmission electron microscope (TEM), which is an excellent complementary research tool. The presence of scanning Raman and IR microscopes (both lab and UVSOR based) provide additional complementary analytical microscopy techniques. Efforts should be made to facilitate multi-technique studies, for example, by developing sharable sample mounting and methods to quickly locate the same spatial regions of samples in the different microscopes.

2.6 Solid State Science (BL1B, BL5U, BL6B, BL7U: Shin-ichi KIMURA, UVSOR)

BL7U and **BL5U**, both dedicated to angle resolved photoemission (ARPES) of surfaces and solids, are the 1st and 2nd most popular beamlines at UVSOR, as judged by usage, ratio of allocated to requested shifts, and numbers of publications in high profile journals. BL7U is among the very best facilities world wide for condensed matter electronic structure studies using low energy photons. Usually researchers turn to beamlines with higher photon energy (>100 eV) if they need additional sampling depth to ensure they are sampling bulk properties. At **BL7U** very low outgoing electron energies are used, as these are also bulk sensitive. The energy resolution of 2 meV (electron and photon combined) is only surpassed by a few other lines in the world. The Apple II insertion device means that the full polarization properties of samples can be explored. A range of outstanding condensed matter science is taking place on BL7U including: detailed studies of Fe-based superconductors; exploration of charge density wave effects at the surface of graphite; investigation of organic conductors. The ongoing development of conventional optical focusing techniques for UV light to achieve sub-micron spot sizes in the 7-9 eV photon energy could lead to some world-unique capabilities which would complement higher photon energy nano-ARPES lines at the ALS (Maestro) and Soleil (Antares). The potential for using such a facility to study laterally heterogeneous surfaces was illustrated with a novel system of electronic phase separation which is suspected to occur in κ-$(Et)_2Cu[N(CN)_2]Br$ on the sub-micron spatial scale. BL7U should invite more international users.

While **BL5U** is a somewhat older ARPES system with lower performance, its higher photon energy range (up to 200 eV) provides a useful complement to BL7U. Planned modifications to improve the performance of BL5U were described, including replacement of the monochromator, which has a resolving power of only 3000, as opposed to the 10,000-50,000 resolving power of BL7U. Although a number of organic materials are being studied with BL7U and 5U, the majority of the science is in the realm of condensed matter physics of semiconductors, metals and correlated electron materials.

BL6B provides light in the IR and THz range. Kimura outlined some exciting instrumentation developments, including his magic mirror which achieves exceptionally large angular collection of bend magnet IR radiation (only exceeded by the mirror array system of the IRENI facility at SRC, Wisconsin), and the recent adoption of a focal plane array detector for far- and mid-IR spectromicroscopy on BL6B. Interesting science using far-IR (THz) to study organic materials at high pressure was presented. However there has been relatively little molecular science using BL6B despite the extensive use of synchrotron IR spectroscopy and spectromicroscopy for molecular science at other SR facilities around the world. Given the activities in organic electronic materials and biosciences at IMS, it would seem there is excellent potential to expand use of BL6B, especially in the mid-IR to visible range where many non-SR scientists are actively using lab based IR spectroscopy and spectromicroscopy. I understand that Assoc. Prof. Furutani (Life and Co-ordination Complex Molecular Science, IMS) is interested in partly-dedicated use of BL6B for bioscience applications. The new program to provide such 'approved program' time (outlined by Kimura at the end of his Friday presentation) seems to be an excellent opportunity to increase molecular science activity at the IR microscope on BL6B. There is also a lot of science which can be advanced using STXM and IR microscopy in a complementary fashion. Development of identical or cross-compatible sample mounting and fiducialization approaches (perhaps linked through the encoded stages of the optical microscope at BL4U STXM) could significantly facilitate that development.

BL1B has capabilities for developing novel coherent THz and THz-VUV experiments using laser slicing with amplitude modulated pulse trains. This is very exciting light source physics with good potential to achieve new physics. Possible molecular science applications of the coherent THz source were outlined in the areas of protein motion and carrier dynamics in Li ion battery and organic Dirac Fermion materials. At present the motivation is clearly exploration of novel instrumentation / light source capabilities. Its impact on molecular science is likely to be limited, at least in the short term.

2.7 Magnetic materials (XAS, XMCD) (BL4B: Toshihiko YOKOYAMA, IMS)

The superconducting magnetic spectroscopy system on **BL4B** is a competitive facility relative to related systems internationally. It has among the highest on-sample magnetic field at SR facilities and has a good degree of flexibility in sample mounting relative to the field and photon polarization such that all aspects of the magnetic properties of samples can be measured. The facility is part of the Nanotechnology Platform Project in Japan, for which funding was recently renewed for a 10 year period. Professor Yokoyama gave overviews of five specific research projects in the surface and thin film magnetism: magnetic properties of Fe islands and nanowires on W(110); Co nanorods on Cu(110)-(2x3)N; γ'FeN/Cu(001); Fe on Si_3N_4/Si(111)-(8x8); VOPc/Si(111). The latter is the only example with a molecular science flavor. In this case, a combination of polarization dependent NEXAFS and V 2p XMCD was used to determine the structure and magnetism. Although there was a significant change in electronic structure and bonding between monolayer and multilayer VOPc, the V 2p XMCD magnetic signature was identical indicating the V 3d character is similar despite the bonding change. All of the examples presented high quality data from very challenging low signal systems. While similar science is being done elsewhere, Professor Yokoyama noted a major advantage of the UVSOR operation was the much lower time pressure which allows for sufficient time to study samples requiring careful *in situ* preparation.

2.8 Photoemission of organic solids (BL8B: Satoshi KERA, Chiba Univ)

BL8B is a public beamline dedicated to ultraviolet photoemission spectroscopy and ARPES of organic solids. The presentation gave a strong motivation for the research of the Chiba group in terms of the need to understand the fundamental principles of molecular assembly in order to control electronic structure and functionality of organic materials for electronics applications. A quantum perspective and the theme of wavefunction spreading was used to interpret recent results on: weak band gap states in fullerene thin films; conduction mechanism and hole-phonon coupling as a limit to charge mobility in pentacene films; band dispersion in rubrene. BL8B is the oldest beamline at UVSOR. Plans to improve the instrumentation (replace the current analyzer with a modern 2D angle-energy electron spectrometer) and move from 8B to 2B were described and motivated by the need for higher performance to enable use of UV-ARPES for momentum space orbital mapping of organic solids. This approach was highlighted by a number of presentations at the recent ICESS12 meeting and is clearly a trend in international science in this area.

2.9a VUV optical properties (BL3B, BL7B: Shin-ichi KIMURA, UVSOR)

BL3B and **BL7B** are dedicated to studies of the

optical properties (reflection, absorbance and luminescence) in the visible – and vacuum UV regions. **BL7B** is an older beamline that has recently been reconfigured to focus on ellipsometry measurements. **BL3B** has recently been moved from BL1B and significantly upgraded to the HOTRLU system which has greatly improved flux (relative to the previous BL1B system), and a smaller spot size by using a Kirkpatrick-Baez focusing system. Research on the UV optical properties of a number of interesting materials was described, including AlN and EBSTO, a layered organic-inorganic system, as well as studies related to calibrating instruments for astrophysics. There is significant international participation and quite high productivity (BL3B & BL7B generated over 20% of all UVSOR publications in the past 5 years), although the publications are rarely in the first rank journals.

2.9b VUV spectroscopy of biological molecules (BL3B, BL7B: Kazumichi NAKAGAWA, Kobe Univ.)

Professor Nakagawa described his program for careful transmission measurements on thin films of the individual amino acids and DNA bases, which are used to generate absolute absorption cross-sections. Results are typically reliable to 5-10%, but often only after a sum-rule normalization correction. The motivation for the work is UV biosensors, and connections to UV damage related to cataracts. However there was no evidence for a direct link to those areas, and the energy range relevant to these issues is only a very small part of the energy range over which the absorption was measured. However, in terms of understanding the fundamental physics and chemistry of radiation damage, such a wide range of spectral studies may be meaningful.

3. General comments about science and future directions for UVSOR

3a. International competitiveness

As outlined in detail above, some beamlines, end-stations and research programs are more internationally competitive than others. Of particular high quality I consider BL3U, BL6U and BL3B.

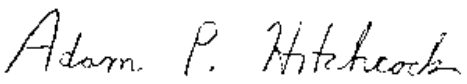
3b. Relevance to molecular science mission

The liquids, electrochemistry, and chemical / photochemical reaction science, as well as the electronic structure (ARPES, XAS, XES) studies of molecular thin films are areas of the most direct relevance to molecular science. There is a strong tradition of gas phase spectroscopy studies at UVSOR which is very relevant to molecular science. However, I was less impressed by the instrumentation and science in this area, than in other areas. Although not mainstream molecular science, the instrumentation and programs in condensed matter electronic structure (ARPES) are very strong and definitely worth continuing.

3c. Role of in-house contributions / future directions

A key aspect of UVSOR is that a large proportion of the scientific direction, instrumentation development, and beamtime is determined by the in house scientists. This is in strong contrast to most other SR facilities, where it is the science and interests of external researchers that is dominant. I consider the exceptional in-house research programs to be a real strength of UVSOR. The quality of the science on the international scale then strongly depends on the quality of the team leaders, the researchers they attract to their teams, and their international collaborations. IMS is fortunate to have some very talented researchers. Relative to other facilities, the size of the UVSOR staff is very small, yet the output is outstanding, from the perspectives of quality, diversity and quantity. Hiring of at least one additional faculty in IMS or UVSOR, at the professor or associate professor level should be (and, I understand, is) a high priority. While the main goal should be to find a dynamic young or mid-career individual with a passion for synchrotron-based research applied to molecular science, if there are equally good candidates, research in the area of nanoscience would build best on the existing instrumentation and strengths of UVSOR.

November 22, 2012



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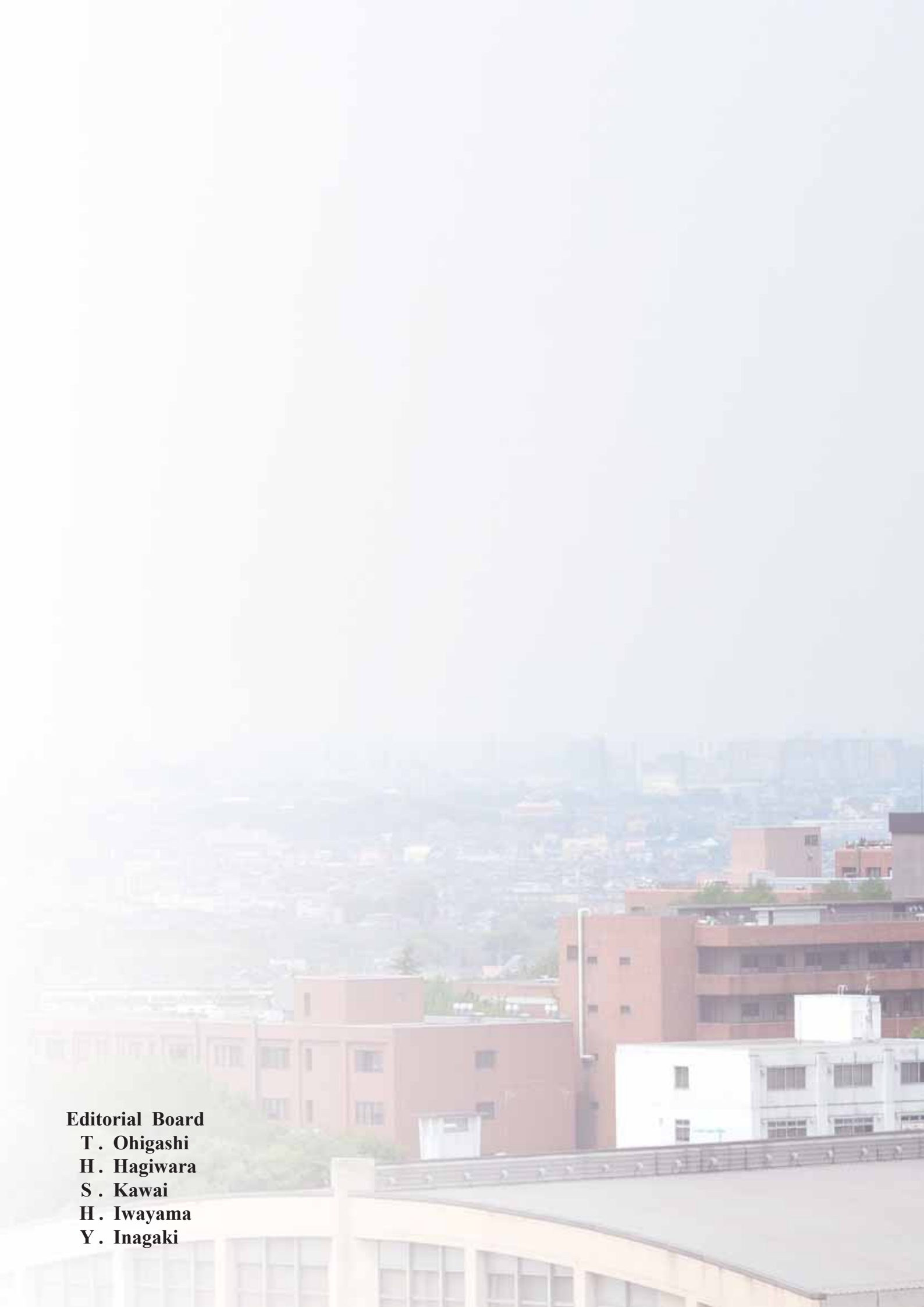

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