

Program

Kobayashi Hall, Kenkyu Honkan Bldg., KEK

December 8 (Thu), 2011

| 8:30 – 9:00 | Opening | Page |
|----------------------|--|-------------|
| 8:30-8:45 | Introduction to the Workshop and Presentation of IUCr SR and XAFS Commissions Strategies toward Standardization <i>- S. Wakatsuki (Photon Factory) 15 min.</i> | 1 |
| 8:45-9:00 | IXAS Strategy toward Standardization <i>-H. Oyanagi (AIST) 15 min.</i> | 2 |
| 9:00-11:45 | S1: Chair: K. Asakura (Hokkaido University) To Establish Standardization of XAFS Set-ups Including Bio-XAFS, Similar to Crystallography I (Standardization of Experimental Methods and Data Formats for Higher-throughput of XAFS experiments). | |
| 9:00-9:30 | Toward the Standardization of XAFS, Transmission mode XAFS Setup <i>- M. Nomura (Photon Factory) 30 min.</i> | 3 |
| 9:30-10:00 | Toward the standardization of BioXAS <i>-I. Ascone (CNRS) 30 min.</i> | 6 |
| 10:00-10:30 | A Step toward Standardization: Development of Accurate Measurements of X-ray Absorption <i>- C. T. Chantler (Melbourne University) 30 min.</i> | 7 |
| 10:30-10:45 | Coffee break 15 min. | |
| 10:45-11:45 | Open Discussion 60 min. Discussion Leader: K. Asakura (Hokkaido University) | |
| 11:45-12:15 | S2 Chair: H. Oyanagi (AIST) To Establish Experimental Protocols for Measurements (e.g. Energy Calibration, Beam Stability, Polarization etc.) to Obtain High Quality Data in Physics, Chemistry and Materials Sciences. | |
| 11:45-12:15 | XAFS Data Collection: an Integrated Approach to Delivering Good Data <i>- S. Diaz-Moreno (Diamond) 30 min.</i> | 8 |
| 12:15-13:00 | Lunch 45 min. | |
| 13:00 – 16:00 | S2 Chair: H. Oyanagi (AIST) (continue) To Establish Experimental Protocols for Measurements (e.g. Energy Calibration, Beam Stability, Polarization etc.) to Obtain High Quality Data in Physics, Chemistry and Materials Sciences. | |
| 13:00-13:20 | A Data Interchange Standard for XAS and Related Spectroscopies <i>- B. Ravel (NSLS) 20 min.</i> | 9 |
| 13:20-13:50 | HDF5, NeXus and Beyond – Approach to a Standard Data Format <i>- V. A. Sole (ESRF) 30 min.</i> | 10 |
| 13:50-14:20 | XAFS Data Library for Standard Data on Model Compounds <i>- M. Newville (University of Chicago) 30 min.</i> | 11 |
| (14:20-14:30) | (Short break 10 min.) | |
| 14:30-15:00 | Imagining a CIF-based XAFS Data Exchange Framework <i>-J. Hester (ANSTO) 30 min.</i> | 12 |
| 15:00-16:00 | Open Discussion 60 min. Discussion Leader: A. Sole (ESRF) and M. Newville (Univ. of Chicago) | |
| 16:00 - 16:15 | Coffee break 15 min. | |
| 16:15-19:00 | S3-I Chair : K. Hodgson (SSRL) Advanced Techniques and Newly Developed XAFS Beamlines with Advance Specifications I : New Development for Existing or New Beamlines: Combining XAFS and Other Techniques (XES etc.). | |

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| 16:15-16:45 | Structural Molecular Biology/XAS Beamline: Experiences at SSRL – <i>B. Hedman (SSRL)</i> 30 min. | 13 |
| 16:45-17:15 | The BioXAS beamlines at the Canadian Light Source – <i>G. N. George (University of Saskatchewan)</i> 30 min. | 14 |
| 17:15-17:30 | Coffee break 15 min. | |
| 17:30-18:00 | Metal Speciation in Biological Systems with XANES and XAFS – <i>P. A. Lay (University of Sydney)</i> 30 min. | 15 |
| 18:00-18:30 | Energy Dispersive XAS: Worldwide Context – <i>S. Pascarelli (ESRF)</i> 30 min. | 16 |
| 18:30-19:00 | Quick XAFS Techniques - Current status and New Challenges at PETRA III – <i>R. Frahm (Bergische Universität Wuppertal)</i> 30 min. | 17 |
| 19:30-21:30 | Banquet at the foyer | |

December 9 (Fri), 2011

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| 9:00-10:30 | S3-II Chair: M. Newville (Univ. of Chicago) Advanced Techniques and Newly Developed XAFS Beamlines with Advance Specifications II. | |
| 9:00-9:30 | An Advanced Beamline for XAS and IR Simultaneous Time Resolved experiments. A new Approach to Characterize Non Equilibrium Phenomena. – <i>A. Marcelli (INFN)</i> 30 min. | 18 |
| 9:30-10:00 | Opportunities and Traps of Hard X-ray Photon-in/Photon-out Spectroscopy – <i>P. Glatzel (ESRF)</i> 30 min. | 19 |
| 10:00-10:30 | Ideas for Assuring Data Quality and Comparability at The New PETRA III EXAFS Beamlines – <i>E. Welter (DESY)</i> 30 min. | 20 |
| 10:30-10:45 | Coffee break 15 min. | |
| 10:45-11:45 | Brief Summary Report I – K. Asakura (Hokkaido University) 20 min. Discussion 40 min. | |
| 11:45-13:00 | Lunch 75 min. | |
| 13:00-13:30 | S4 Chair: S. Pascarelli (ESRF) XAFS in Green Technology (Science and Technology Related to Environments and Energy Generations/Savings): Requirements for Industrial Use. | |
| 13:00-13:30 | Insight through in situ XAS studies of Catalytic materials – <i>G. Sankar (University college London)</i> 30 min. | 21 |
| CANCELLED | <i>In situ</i> structural studies of catalysts under high gas pressure environment – <i>O. V. Safonova (PSI)</i> 30 min. | 22 |
| 13:30-14:35 | S5 Selected Poster Talks Coordinator: H. Abe 65 min. | |
| | Single Crystal XAS Studies on Metalloprotein Intermediates – <i>R. Sarangi (Stanford University)</i> | 23 |
| | T-REX for advanced QEXAFS data analysis – <i>J. Stötzl (Bergische Universität Wuppertal)</i> | 24 |
| | In situ Time-resolved XAFS Study of the Formation Mechanism of Rh NPs in the Presence of Quaternary Ammonium Bromide – <i>H. Asakura (Kyoto University)</i> | 25 |
| 14:35-14:50 | Short break 15 min. | |
| 14:50-15:50 | Brief Summary Report II – I. Ascone (CNRS) 20 min. Open Discussion 40 min. | |
| 15:50-16:10 | Coffee break 20 min. | |
| 16:10-17:50 | S6 Chair: H. Abe | |

| New Challenges in XAFS Research and Requirements on Light Sources and Beamlines | | |
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| 16:10-16:50 | Recent Developments with the LCLS X-ray FEL at SLAC and Prospects for Future Science - K. O. Hodgson (SSRL) 40 min. | 26 |
| 16:50-17:50 | Panel Discussion 60 min. Future prospects and demands on XAFS beamlines Discussion leaders: Moderator: P. Lay (from Asia-Oceania) Panellist: S. Pascarelli, P. Glatzel (from EU), M. Nomura, B. Hedman, G. George (from North America) | |
| 18:00-20:15 | Poster session with a buffet-style dinner at the foyer | |
| 20:15-20:30 | Poster Awards Ceremony 15 min. | |
| | Presenter: I. Ascone (CNRS), Support presenter: H. Abe (KEK) | |
| 20:30-20:45 | Summary Report & Closing 15 min. | |
| 21:00-23:00 | Closed Night Session for Summary Report Preparation | |

Poster Presentation

| Poster # | Title/Presenter | Page |
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| P-01 | <i>In situ</i> Observation of Reduction Reactions of Iron Oxides by XAFS [1]. - T. Takayama (<i>Nippon Steel Corp.</i>) | 27 |
| P-02 | Understanding the Nature of the Kinetic Process in a VO ₂ Metal-Insulator Transition - Q. Liu (<i>University of Science and Technology of China</i>) | 28 |
| P-03 | Single Crystal XAS Studies on Metalloprotein Intermediates - R. Sarangi (<i>Stanford University</i>) | 23 |
| P-04 | New Development of 1W1B-XAFS Station in Beijing Synchrotron Radiation Facility - Z. Jing (<i>Institute of High Energy Physics</i>) | 29 |
| P-05 | Time-resolved XAS beamline at SLRI - P. Chirawatkul (<i>Synchrotron Light Research Institute</i>) | 30 |
| P-06 | XANES Database in the CK, NK, and OK Regions of Standard Organic Compounds and Metal Compounds for Chemical Analysis - Y. Nakayasu (<i>University of Hyogo</i>) | 31 |
| P-07 | Total-Electron-Yield (TEY) Soft X-Ray Absorption Spectroscopy of the sp ² /sp ³ -Carbon Mixtures; Relationship between the TEY Efficiency and Electrical Conductivity - Y. Muramatsu (<i>University of Hyogo</i>) | 32 |
| P-08 | <i>In situ</i> Time-resolved XAFS Study of the Formation Mechanism of Rh NPs in the Presence of Quaternary Ammonium Bromide - H. Asakura (<i>Kyoto University</i>) | 25 |
| P-09 | Continuous Observation by Dispersive XAFS Technique for Catalytic Reaction - D. Matsumura (<i>Japan Atomic Energy Agency</i>) | 33 |
| P-10 | XAFS measurements from Mg to Zn K-edges at Beamline 8 of Siam Photon Laboratory - W. Klysubun (<i>Synchrotron Light Research Institute</i>) | 34 |
| P-11 | Time-resolved <i>In situ</i> XAFS Studies on Formation and Oxidation of Pd-Zn nanoparticles on ZnO - Y. Uemura (<i>KEK-PF</i>) | 35 |
| P-12 | Determination of Electronic and Geometric Structure of Molybdenum in Molybdenum-based Catalysts using L-edge X-ray Absorption Spectroscopy - C. Kongmark (<i>Synchrotron Light Research Institute</i>) | 36 |
| P-13 | Weak Interaction Effect Study of Blue Copper Protein with XAS - T. Yamaguchi (<i>Ibaraki University</i>) | 37 |
| P-14 | XAS Studies on Electronic Structure of Metal Sites in a Blue Copper Protein, Plastocyanin form Fern <i>Dryopteris crassirhizoma</i> | 38 |

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| | - <i>H. Togashi (Ibaraki University)</i> | |
| P-15 | Status of the Toyota Beamline at the SPring-8 - <i>Y. Nishimura (Toyota Central R&D Laboratories, Inc.)</i> | 39 |
| P-16 | T-REX for advanced QEXAFS data analysis - <i>J. Stötzl (Bergische Universität Wuppertal)</i> | 24 |
| P-17 | Dynamic Investigation of Photoinduced Phase Transition by Picosecond Time-resolved XAFS - <i>S. Nozawa (KEK-PF)</i> | 40 |
| P-18 | Observation of the $^3\text{MLCT}$ state of $[\text{Ru}^{II}(\text{bpy})_3]^{2+}$ by picosecond Time-resolved Ru K-edge XAFS - <i>T. Sato (KEK-PF)</i> | 41 |
| P-19 | Upgrade of the ESRF X-ray Absorption Spectroscopy Beamlines: The general purpose EXAFS beamline BM23 <i>O. Mathon (ESRF)</i> | 42 |
| P-20 | Upgrade of the ESRF X-ray Absorption Spectroscopy Beamlines: The Energy Dispersive EXAFS Beamline ID24 <i>O. Mathon (ESRF)</i> | 42 |
| P-21 | Upgrade of the ESRF X-ray Absorption Spectroscopy Beamlines: The scientific case <i>S. Pasquarelli (ESRF)</i> | 43 |
| P-22 | High-accuracy Measurements of the X-ray Mass-attenuation Coefficient of Copper - <i>C. T. Chantler (Melbourne University)</i> | 44 |
| P-23 | XAFS and XANES Analysis: A study in errors - <i>C. T. Chantler (Melbourne University)</i> | 45 |

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