XAFS13 Conference Overview

Gordon Brown – Stanford University and SSRL

The 13th International Conference on X-ray Absorption Fine Structure (XAFS) was held at Stanford University on July 10-14, 2006 and was attended by about 400 scientists representing 22 countries. Almost 100 oral presentations were made, including seven plenary lectures, and about 430 posters were presented during four poster sessions. The plenary lectures included two on recent advances in theoretical interpretations of X-ray Absorption Near Edge Structure (XANES) spectra, one on XAFS spectroscopic characterization of the manganese cluster in Photosystem II, one on the electronic and molecular structure of liquids as studied by picosecond XAFS, one on XAFS spectroscopy and x-ray fluorescence imaging studies of corrosion of glasses of different ages, including stained glasses from some of the great cathedrals of Europe, one on the application of XANES spectroscopy and photoemission electron microscopy to nanobiology, and one on the scientific career of Dale Sayers, one of the pioneers in XAFS spectroscopy who recently passed away. The scientific sessions included the Dale Sayers Symposium as well as the following disciplinary areas: (1) biology (active sites in isolated systems and *in-situ* imaging), (2) catalytic processes, (3) novel and unusual experimental methods, (4) modeling and data analysis approaches, (5) magnetic properties and systems, (6) time-resolved spectroscopy, (7) materials studies, (8) chemistry (processes and systems), (9) theory, calculations, and modeling, (10) environmental applications, (11) developments in XAS theory, (12) actinides in the environment, (13) *in-situ* XAS studies, (14) XAS and nanomaterials, and (15) biomedical XAS applications.

The conference co-chairs responsible for the overall organization of XAFS13 were Profs. Britt Hedman, Piero Pianetta, and Keith Hodgson of the Stanford Synchrotron Radiation Laboratory (SSRL). Conference organization and infrastructure needs were ably provided by a number of SSRL staff members, including Stephanie Carlson, Lisa Dunn, Cathy Knotts, Michelle Montalvo, Ann Mueller, Jennifer Peck, Jackie Robleto, Amy Rutherford, Todd Slater, and Michelle Steger. Financial support was provided by Stanford University, a number of US National Laboratories and international light sources [including the Advanced Photon Source (APS-Argonne National Lab), the Advanced Light Source (ALS-Lawrence Berkeley National Lab), the National Synchrotron Light Source (NSLS-Brookhaven National Laboratory), Stanford Synchrotron Radiation Laboratory (SSRL), Stanford Linear Accelerator Center (SLAC), Synchrotron Radiation Center (SRC), SOLEIL Synchrotron, Hamburger Synchrotronstrahlungslabor (HASYLAB), Berliner Elektronenspeicherring – Gesellschaft fur Synchrotronstrahlung (BESSY), the Canadian Light Source (CLS), and the National Synchrotron Radiation Research Center (NSRRC)], as well as by the following commercial exhibitors: Brush-Wellman Electrofusion Products, Canberra, Kohzu America, Inc., VG Scienta, Inc., and XIA LLC.

There were a number of highlights at the XAFS13 Conference. One involved the tremendous advances being made in blending theory and experiment. An example of these advances is the recent oxygen K-edge XAS and X-ray Raman Scattering (XRS) studies of the structure of bulk water and the interpretation of these spectra using state-of-the-art density functional theory, as reported in the plenary lecture of Lars G.M. Pettersson of Stockholm University. As one conferee put it, it's amazing that a small pre-edge feature in the oxygen K-edge XAS spectrum of liquid water has turned the water community upside down in its understanding of the average structure of water, the most common solvent on Earth. Another example is the advance in understanding of pre-edge features of 3d-transition metal ions using multiplet theory, as discussed by Frank deGroot of the University of Utrecht. Also

highlighted by Vittal Yachandra of Lawrence Berkeley National Laboratory was the new understanding provided by XAFS spectroscopy of the photosynthetic water-oxidizing complex that contains a unique Mn_4Ca cluster. Another highlight involved discussion of new methods, particularly X-ray Raman Scattering, Resonance Inelastic X-ray Scattering (RIXS), quantitative structural analysis of matter using XANES spectroscopy, and ultrafast methods that allow time-resolved studies of matter at the picosecond time scale and below. Another area in which impressive advances have been made since XAFS12 was held in Malmö, Sweden in 2003 are new applications of XAFS and related methods in biology, chemistry, materials science (including magnetic and nanomaterials), environmental science, condensed matter physics, and medical science. The enormous growth in applications of XAFS spectroscopy in particular and synchrotron radiation methods in general to these and other areas of science and engineering was emphasized by discussions of a number of new synchrotron radiation sources, either nearing completion or in the final planning stages, including the Canadian Light Source (Saskatoon, Saskatchewan, Canada), Diamond Light Source (Didcot, Oxfordshire, UK), Synchrotron SOLEIL (Saint-Aubin, France), Australian Synchrotron (Boomerang 20) (Melbourne, Victoria, Australia), and the Spanish Light Source (ALBA) (Barcelona, Spain).

In addition to 20 thematic oral sessions and four general poster sessions, the XAFS13 Conference featured a special symposium honoring Dale Sayers, with talks by a number of his friends and scientific collaborators. Dale was one of the three pioneers of XAFS spectroscopy, all of whom have remained very active in its applications. At the time of his death in November 2005, Dale was actively pursuing new medical imaging methods using synchrotron radiation for applications in mammography. His two mentors, Farrell Lytle and Ed Stern, also remain very active, with Farrell using XAFS methods to study desert varnishes, and Ed Stern using XAFS to study ultrafast changes in thin metal films excited by lasers.

There were three awards presented in a ceremony the same afternoon. The Edward Stern International XAFS Society (IXS) Outstanding Achievement Award was given jointly to Calogero R. Natoli, INFN, Italy and John J. Rehr, University of Washington, USA in recognition of their fundamental contribution for the development of XAFS theory (presented by Ed Stern). The IXS Farrel Lytle Outstanding Young Scientist Award for Theory or Instrumentation was given to Pieter Glatzel, ESRF, France in recognition of his contribution in developing XAFS-related techniques such as x-ray emission spectroscopy, resonant and non-resonant x-ray scattering (presented by Farrel Lytle). The IXS Dale Sayers Young Scientist Award for Applictions of XAFS was given to Jan-Dierk Grunwaldt, ETH, Switzerland in recognition of his contribution in the application of XAFS in catalysts and in the study of chemical reactions; this award was presented by Anne Sayers.

Overall, the XAFS13 Conference was a highly successful gathering of scientists who shared their new theoretical and experimental developments and a broad range of applications of XAFS spectroscopy. The large number of young scientists attending the meeting was impressive and bodes well for the future of this method and its applications. The presentations and lively discussions at XAFS13 made clear that since its introduction in 1971 by Sayers, Stern, and Lytle, XAFS spectroscopy has become a mature methodology with exciting applications in many areas of science and engineering. The 276 papers published in this proceedings volume attest to this statement. We look forward to the next international gathering of XAFS aficionados (XAFS14) in Camerino, Italy in Summer 2009.