Jingguang Chen (U. Delaware) demonstrated the power of soft x-ray absorption spectroscopy in elucidating surface reaction mechanisms in catalysis. He showed data probing novel hydrogenation chemistry on nickel oxide monolayer films and, using data from early transition metal carbides, highlighted the power of NEXAFS to correlate data from model surfaces with that from realistic catalytic materials. He concluded by briefly discussing the in situ capabilities of NEXAFS using fluorescence yield with the example of lithium nickel oxides in methane oxidation.

The session closed with a talk by Jim Penner-Hahn (U. Michigan). He presented recent results on the local structure around the active zinc site in enzymes – the talk highlighted how new biochemistry can be learned using traditional x-ray spectroscopy.

In other business of the NSLS Users’ Meeting, elections for the Users’ Executive Committee members took place. Elected were Steve Almo (Albert Einstein College of Medicine), Dan Fischer (NIST), and Tony Lanzirotti (U. Chicago). Also announced were the results from the elections for the Special Interest Group (SPIG) representatives, the winners being Paul Stevens (Exxon-Mobil Research & Engineering) for Industrial Users; Vince Harris (NRL) for EXAFS; Mike Dudley (SUNY Stony Brook) for Topography; Dave Mullins (ORNL) for UV/Photoemission; Mike Becker (Biology, BNL) for Biological Scattering & Diffraction; Mark Furhmann (Env. Sci., BNL) for Imaging; Lisa Miller (NSLS, BNL) for Infrared; Mahbub Khandaker (Jefferson Lab) for Nuclear Physics; Cecilia Sanchez-Hanker (NSLS, BNL) for Students/Postdocs; John Sutherland (Biology, BNL) for Time Resolved Spectroscopy; and Peter Stephens (SUNY Stony Brook) for X-ray Scattering & Crystallography.

The day ended with the conference banquet, which was held on-site with the theme of a Hawaiian luau. The cafeteria at Berkner Hall was transformed into an island paradise with tropical decorations and music. Attendees truly got into the theme: colorful Hawaiian shirts were worn by many, and leis were presented as one entered “the island.” There was entertainment in the form of Hawaiian music, dancers, and a fire dancer – along with some entertaining dancing by some of the attendees!

Environmental Molecular Sciences Workshop
May 21, 2001
Richard Reeder (SUNY, Stony Brook)
Tony Lanzirotti (U. of Chicago)

This year’s Environmental-Molecular Sciences Workshop was held as part of the National Synchrotron Light Source’s Annual Users’ Meeting on May 21, 2001. Organized by Tony Lanzirotti (GSECARS, U. Chicago) and Rich Reeder (Geosci. Dept., SUNY Stony Brook), this is the second in what is hoped will be an annual event. Eight speakers presented research conducted at beamlines at the NSLS. Doug Hunter (Savannah River Tech. Center) showed how interpretation of chemical processes in contaminated soils often requires both bulk- and micro-sample analysis. To illustrate this he presented bulk EXAFS (X23A2), microbeam XANES and XRF (X26A), and FTIR and Raman data on plutonium and chromium contaminated tuffs and uranium contaminated soils.

Don Sparks (Dept. of Plant and Soil Sci., U. Delaware) touched on the similar issue of how to relate field observations made for contaminated soils to molecular and atomic scale interactions. He presented data from zinc and arsenic contaminated sites, emphasizing that proper interpretation requires the use of multiple techniques such as EMPA, XRD, EXAFS (X11), and microbeam XRF and XANES (X26A).

Jay Brandes (Marine Sci. Inst., U. Texas-Austin) showed how soft x-ray transmission microscopy (X1A) is used to evaluate sources of carbon in marine environments. These samples, some collected at over 3400 meters depth in the ocean, are dominated by remnants of marine organisms and provide unique insights into the sources of organic carbon at these depths. He illustrated how sub-micron spatial resolutions are needed to precisely evaluate the composition of these environmental materials.

Jeff Gillow (Dept. of Environ. Sci., BNL) presented research on how bacterial organisms can affect the migration mechanisms of actinides in the environment. In particular, how colloidal mobilization by bacteria became an issue at the Waste Isolation Pilot Plant (WIPP) in NM. Based on SEM-TEM-EDS analyses, EXAFS results from X11, and STXM data from X1A, Jeff showed
that bacterial species such as Halomonas and Clostridium effectively complex uranium within their cell structure.

Murthy Vairavamurthy (Dept. of Environ. Sci., BNL) showed how x-ray absorption spectroscopy (X19A) is used to evaluate the role S and N in forming macromolecules and in driving organic matter transformations from bio- to geo-polymers. He demonstrated that catalysis and abiotic transformations are important mechanisms in these processes.

John Parise (Geosci. Dept., SUNY Stony Brook) presented a discussion of state-of-the-art developments in the application of micro-beam XRD to earth science materials (X26A). He demonstrated how such spatially resolved (10 micron) analyses can be coupled with simultaneous XRF and XANES analysis to provide a more complete understanding of the geochemical environment of a material.

Andreas Scheinost (Inst. of Terrestrial Ecology, ETH) presented data from a number of zinc contaminated sites and emphasized that spatially resolved XAS and XRF are almost a requirement to understanding the heterogeneous distribution of contaminants in soils. He demonstrated using principal component analysis on directly sampled materials and samples treated by selective sequential extraction that the zinc distribution in these soils reflects a diverse mineralogy at micron scale.

Lastly, Richard Osgood (BNL and Columbia U.) presented results that provide fundamental first-order data on the nature of the sub-surface transport of metal oxides by looking at reactions occurring at metal-oxide/water-interface model surfaces (Fe, Fe₂O₃, Fe₃O₄, etc.). Such minerals (e.g. hematite) are known to promote the reduction Cr⁶⁺ and dehalogenate compounds such as CCl₄. Combining a variety of analytical tools (UHVSTM/AFM, AES/SIMS, NEXAFS, and XPS) they were able to identify the reaction products formed on the metal surface and how these surface species are desorbed.

It’s clear that the excellent turnout for this year’s workshop emphasizes the need for ongoing interaction between environmental researchers in using synchrotron sourced facilities. Virtually all the speakers emphasized the need to apply multiple analytical techniques in evaluating environmental problems. There was also a common feeling that there is a need for improved spatial resolutions in synchrotron based XRF, XAS, and XRD analysis. Hopefully, future workshops will act to promote the exchange of new ideas, attract new environmental researchers to these facilities and provide a forum to stimulate innovations in techniques and methodologies.

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**Frontiers in Structural Biology at High-Brightness X-Ray Sources Workshop, May 21, 2001**

*Mike Becker and Lonny Berman (BNL)*

The “Frontiers in Structural Biology at High-Brightness X-ray Sources” Workshop held at Brookhaven National Laboratory on May 21st focused on (1) evolving X-ray structural methods in biology (single particles, monolayers, macromolecular folding, and other time-dependent phenomena) that depend on current high-brightness synchrotron sources, and that may be expected to undergo even greater advances with future potential higher-brightness, pulsed X-ray sources, such as hard X-ray Free Electron Lasers (FELs) or Photoinjected Energy Recovery Linacs (PERLs), and (2) new or recent structures of some extremely important membrane proteins by current X-ray methods, which typically require synchrotron beamlines for satisfactory structure solution, and which are a class of proteins that are notoriously difficult for overall structure determination by any method.

The morning session, chaired by Prof. Caroline Kisker of the State University of New York at Stony Brook (SUNY/SB), presented several structures for which, only a decade ago, it was almost unforeseeable that structures of such biological importance would be solved this early in the new century. The first speaker of the morning was Dr. Peter Orth, who spoke on the crystal structure of the Photosystem-II reaction center (PS-II), based upon work done in the laboratory of Prof. Wolfram Saenger of the Freie Universitât in Berlin. This structure represents the Holy Grail for many in photosynthesis, as PS-II is the site of water splitting and oxygen evolution, which generates molecular oxygen on Earth, and is of potential importance for design of solar energy devices. The complex that was crystallized consisted of at least 17 subunits. The structure was determined for a non-crystallographic dimer to a resolution of 3.8 Å; at this resolution, not all of the subunits could be assigned, but Cα carbons could be modeled for almost 2,500 residues, and many chromophores could be assigned. Some of the most exciting results were finding that the 4 manganese atoms that form the catalytic site for water oxidation and oxygen evolution re-