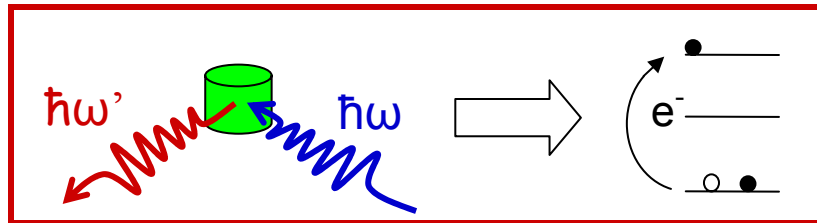


Inelastic X-ray Scattering and Advanced Spectroscopy Facility for SPEAR3

Workshop at SSRL Users' Meeting, October 8, 2003



The workshop '[Inelastic X-ray Scattering and Advanced Spectroscopy Facility for SPEAR3](#)' was held on October 8, 2003 in conjunction with the annual SSRL Users' Meeting. [Twenty-seven participants were registered including eight speakers.](#)



The meeting was started with [a talk by Uwe Bergmann](#) (Stanford Synchrotron Radiation Laboratory), who introduced the various techniques that will be carried out at the proposed facility: X-ray Raman scattering (XRS), resonant inelastic x-ray scattering (RIXS), selective x-ray absorption (S-XAS) and x-ray emission spectroscopy (XES).

XRS will widen the range of absorption spectroscopy on low Z samples traditionally performed in the soft x-ray range, to systems and sample conditions where the penetration of a hard x-ray probe is essential. XRS can thus provide unique new insight for, e.g., studies of carbonaceous systems related to fossil fuels and hydrogen storage under in-situ conditions, water and aqueous systems in ambient and extreme conditions, high pressure phases of gases and the formation of methane hydrates.

Three talks very mainly concerned with XRS. First, Prof. Anders Nilsson (Stanford University/Stockholm University) reported on '[New perspective on structure and bonding in water using XAS and XRS](#)' showing results on studies of the local water structure performed at ambient and supercritical conditions. Dr. Choong-Shik Yoo, (High Pressure Physics group at

Lawrence Livermore National Laboratory) presented a talk on [‘Needs for advanced x-ray microprobes to study crystal and electronic structures of solids at high pressures’](#) where he elucidated on the fascinating possibilities of studying the electronic structure of 2p molecular solids at high pressure using XRS, as well as pressure induced high-spin to low-spin transitions of 3d metals using XES and RIXS. Finally, Dr. Oliver Mullins (Schlumberger-Doll Research) presented the talk [‘Asphaltenes and Polycyclic Aromatic Hydrocarbons’](#) focusing on the structural studies of these systems by spectroscopic techniques including XRS. Such studies will be at the core of his planned ‘Petroleomics’ initiative aimed at the understanding of properties of crude oil constituents through structure determination with the aim of efficient resource utilization.

RIXS spectroscopy is an advanced technique to study in detail the local electronic structure and spin states of, e.g., 3d transition metal compounds with hard x-rays. As compared to conventional K-edge spectroscopy it can better isolate lowest unoccupied molecular orbital (LUMO) resonances and has less lifetime broadening along the energy transfer axis. Furthermore it provides L-edge/M-edge like information. S-XAS, such as site-selective EXAFS combines the chemical sensitivity of XES with EXAFS to provide more detailed structural information in mixed valence systems. XES contains chemical and structural information complementary to XANES. All of these techniques are valuable in the study of a wide range of systems including man-made and bio catalysts as well as correlated systems.

Prof. Frank de Groot (Utrecht University) reported on [‘Applications of RIXS in catalysis and magnetism’](#) where he gave a detailed review of experimental and theoretical work on RIXS, XES and S-XAS of 3d transition metal compounds. Prof. James Penner-Hahn (University of Michigan) discussed [‘Unsolved problems in biology – what can advanced x-ray spectroscopy contribute?’](#). He listed important metalloproteins, and showed how conventional and advanced x-ray spectroscopy can be applied to study these systems. RIXS and XES were mentioned as potential tools to study the electronic structure even of so-called ‘problem’ metals with closed outer shell. Dr. Vittal Yachandra (Lawrence Berkeley National Laboratory) reported on [‘New x-ray techniques to study the Mn complex involved in photosynthetic water oxidation’](#). He discussed the decades long intensive studies of this arguably most important of all bio-catalysts and how XES, RIXS and high-resolution EXAFS can help to solve the question of: How plants oxidize water? Finally, a look to the longer term future was given by Dr. Kelly Gaffney (Stanford Synchrotron Radiation Laboratory), who presented the talk [‘Time Resolved Studies of Chemical Kinetics and Dynamics at the Linac Coherent Light Source \(LCLS\)’](#). He introduced the field of ultra-fast spectroscopy and the potential applications of XRS, RIXS and XES at the LCLS, where begin of construction is planned for 2006.

The workshop was concluded with a reception at the SLAC auditorium and the discussions continued through the next two days of the User’s Meeting. The participants expressed great interest and enthusiasm regarding the research possibilities at the proposed facility. From a first questionnaire to the participants the following preliminary parameters were obtained:

energy range:	> 4 keV
energy resolution:	0.1 – 1.0 eV (one case 0.05eV, one case ~10 eV)
beam size:	10*10 μm^2 (> 100 GPa pressure) up to 1 * 2 mm^2
insertion device:	small Gap undulator of type U20 (small beam size)
sample environment:	diamond anvil cells, He cryostat, furnace (<1000K), in-situ cells, electro magnet