Applications of

Synchrotron Radiation

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Applications

Materials Research

Basic understanding of semiconductors, metals, superconductors, alloys, elementary excitations, electronic structure, phase equilibrium, actinide chemistry, . . .

Photoelectron Spectroscopy, EXAFS,
Small angle scattering, powder diffraction, . . .

Surface Science

Structure of clean surfaces, ultra-thin films, chemisorption complexes, interfacial junctions, dynamic and kinetic properties of surfaces, growth modes of thin films, . . .

UV Photoemission Spectroscopy (UPS) (Angle-resolved, spin resolved)

Polymers

Structure-property relationships
Small Angle Scattering (SAS)

Applications (continued)

Atomic, Optical, Molecular Physics and Chemistry

Vibration/rotation spectroscopy
Infrared microspectroscopy
Chemical dynamics

Molecular Environmental Science

Study of environmental contaminants

- molecular structure, composition, oxidation state, reaction mechanisms
- stability, toxicity, mobility, bioavailability, SPECIATION

Geosciences

Mineral interfaces, compositional variations and coordination chemistry of materials at high temperature and pressure in the earth's crust, amorphous geological materials, mineral phases and phase transitions at high temperature and pressure, . . .

EXAFS, XANES, IR Spectroscopy; Laser-heated diamond anvil cells

Microscopy

IR, Soft x-ray, hard x-ray

Applications (continued)

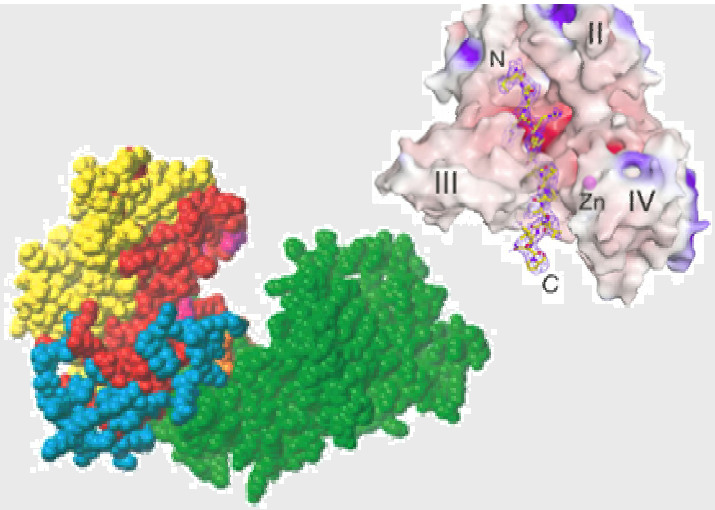
Structural Molecular Biology (Macromolecular crystallography)

- Determination of the 3-dimensional structure of proteins
- Elucidating biological pathways
- Drug design

MAD technique makes use of tunability of synchrotron radiation

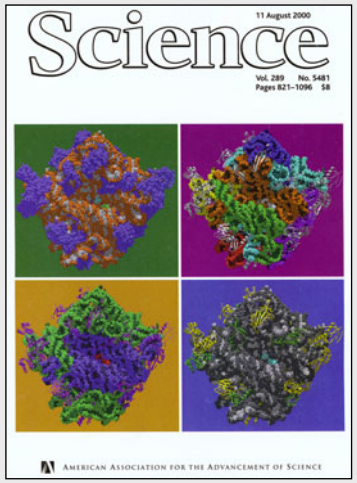
Sequencing of the human genome has led to the need to understand the structure and function of tens of thousands of proteins

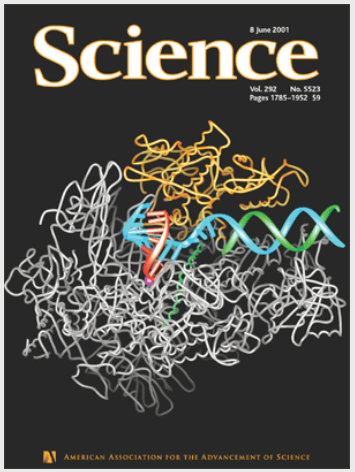
Research Highlights from the Light Sources



Countering Bioterrorism. This past year, using the NSLS, SSRL and APS, researchers have determined the structures of two of the three components that constitute the anthrax toxin: proteins called Lethal Factor and Edema Factor. These structures give molecular insight into how anthrax causes infection and directly guide development of new drugs to defeat the anthrax threat.

Understanding the Molecular Machines of Life. All cells contain remarkable cellular "machines," that decode genes to make proteins. Using data from each of the four synchrotrons, scientists have now determined the structures of two of these remarkable multi-component complexes (called polymerase and ribosome). Besides the remarkable discovery, these structural insights are leading to more effective strategies for designing new antibiotics.



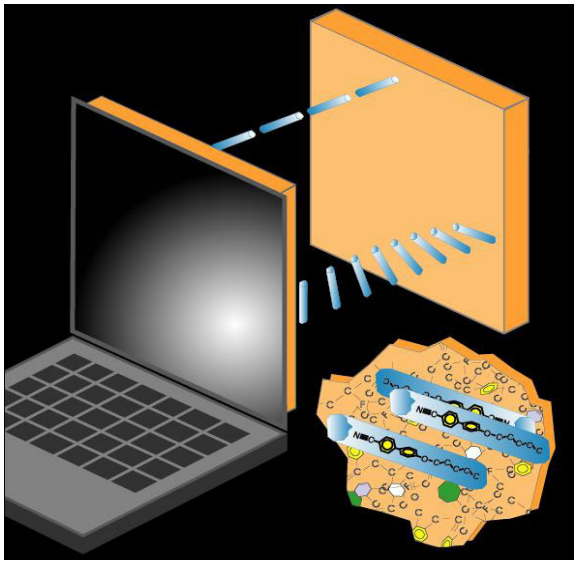


Synchrotron Studies Used to Guide Development of New Process for Manufacture of Flat Panel Displays

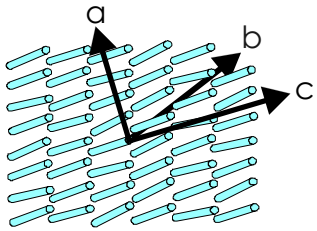
Today's laptop computers utilize flat panel displays where the light transmission from the back to the front of the display is modulated by orientation changes in liquid crystal (LC) molecules. One of the key steps in the manufacture of the displays is the alignment of the liquid crystal molecules in the display. Today this is done by mechanical rubbing of two polymer surfaces and then sandwiching the LC between two such surfaces with orthogonal rubbing directions. Over the past years a great challenge of this $10 billion/year industry has been to devise an alternative method of liquid crystal alignment. The rubbing process is plagued with contamination issues and the polymer film is deposited by a wet process that is incompatible with high-tech manufacturing techniques. The development of a new alignment technology, however, has been impeded by the fact that the origin of LC alignment has remained a mystery since its discovery in 1907.

- Polarization and surface sensitive spectroscopy measurements at SSRL by IBM scientists have been used to solve this puzzle.

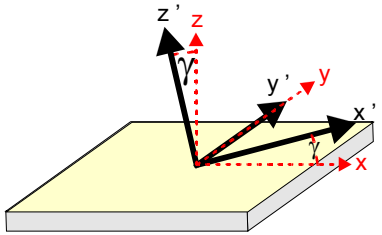
- The understanding of the molecular alignment mechanism for rubbed polymer surfaces has directly led to the development of alternative alignment materials and processes which are discussed in three patents and described in *Science* **292**, 2299 (2001).



Liquid crystal orientation



Molecular surface orientation

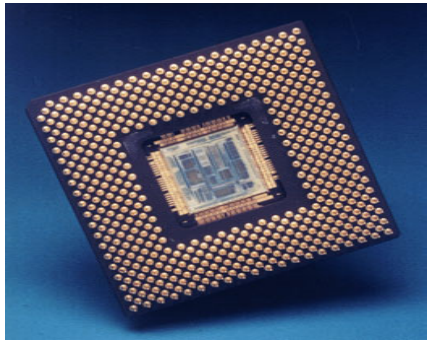


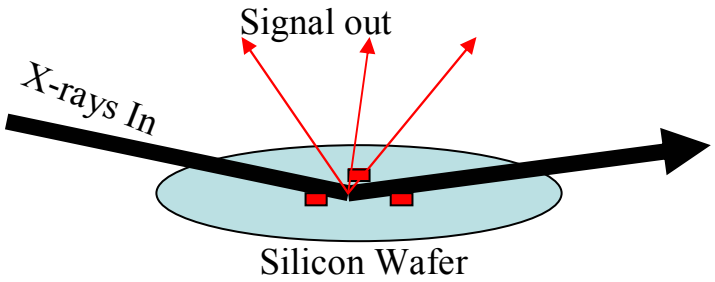
Ultra-Sensitive Analysis of Metal Contamination on Silicon Wafer Surfaces

- Increasing the speed and complexity of integrated circuits requires advanced processes that put extreme constraints on the level of metal contaminants on silicon wafer surfaces.

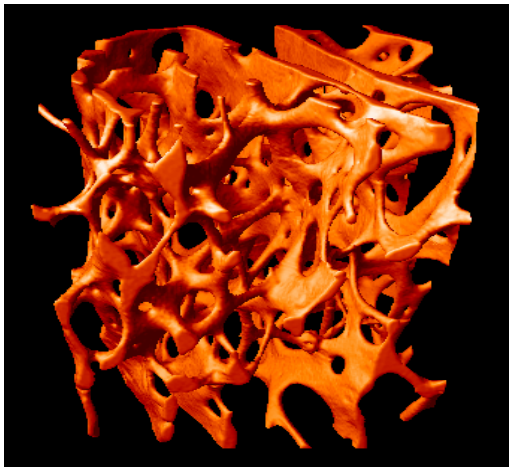
- Synchrotron radiation from SSRL has been used to excite x-ray fluorescence from the metal contaminants with sensitivities as low as one metal atom per 107 silicon atoms. This is 100x better than conventional techniques.

- This sensitivity meets the requirements of the Sematech Roadmap well into the 21st Century and the facility is being used regularly by the semiconductor industry.





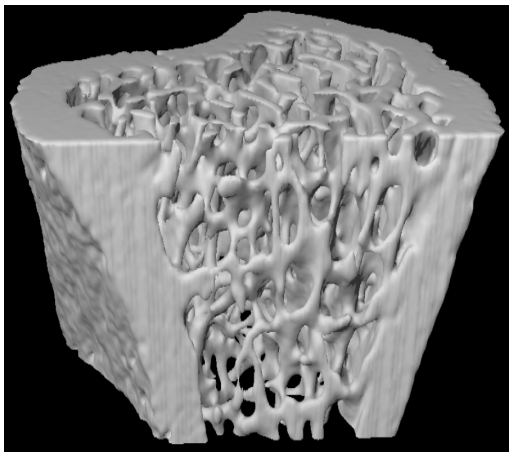
Osteoporosis Research - Understanding Loss of Bone Mass



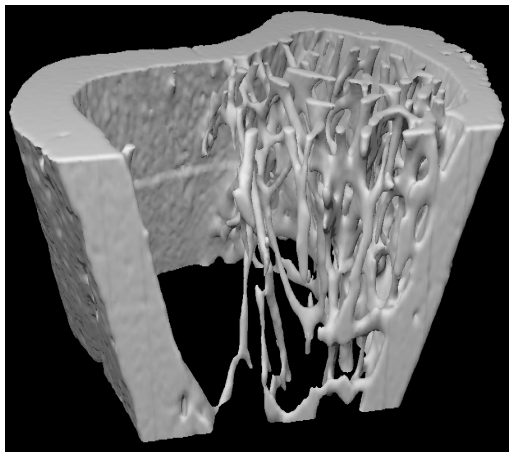
X-ray tomograph of trabecular bone in the human femoral neck taken with synchrotron radiation by LLNL scientists using synchrotron radiation at SSRL

Osteoporosis is a major public health problem

- **1.3 million osteoporotic fractures each year**
- **50% of women over 70 have had at least one fracture**
- **a disease which strikes without warning**
- **responsible for more deaths than breast cancer**



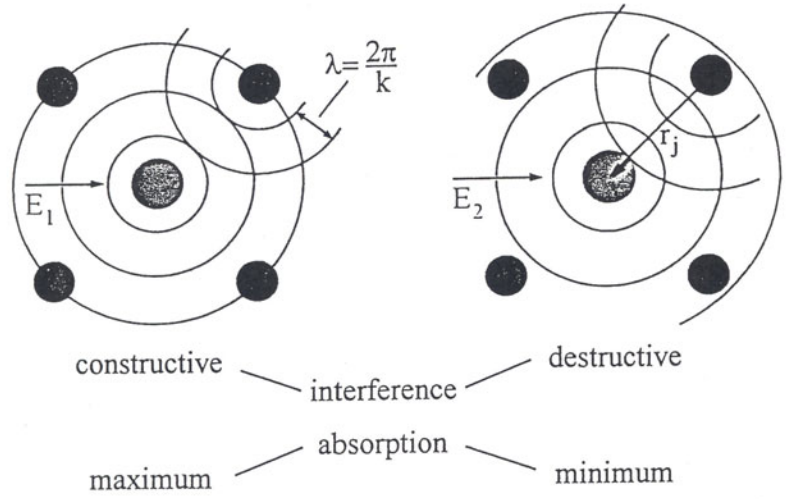
before estrogen loss



after estrogen loss

Estrogen deficiency induces rapid bone loss and altered architecture. This can be visualized in living beings using non-invasive x-ray synchrotron tomography imaging. The image above is from a rat taken under sedation.

EXAFS = Extended X-ray Absorption Fine Structure



Wavenumber of photoelectrons:

$$k = \sqrt{\frac{2m_e}{\hbar^2} \cdot (E - E_0)}$$

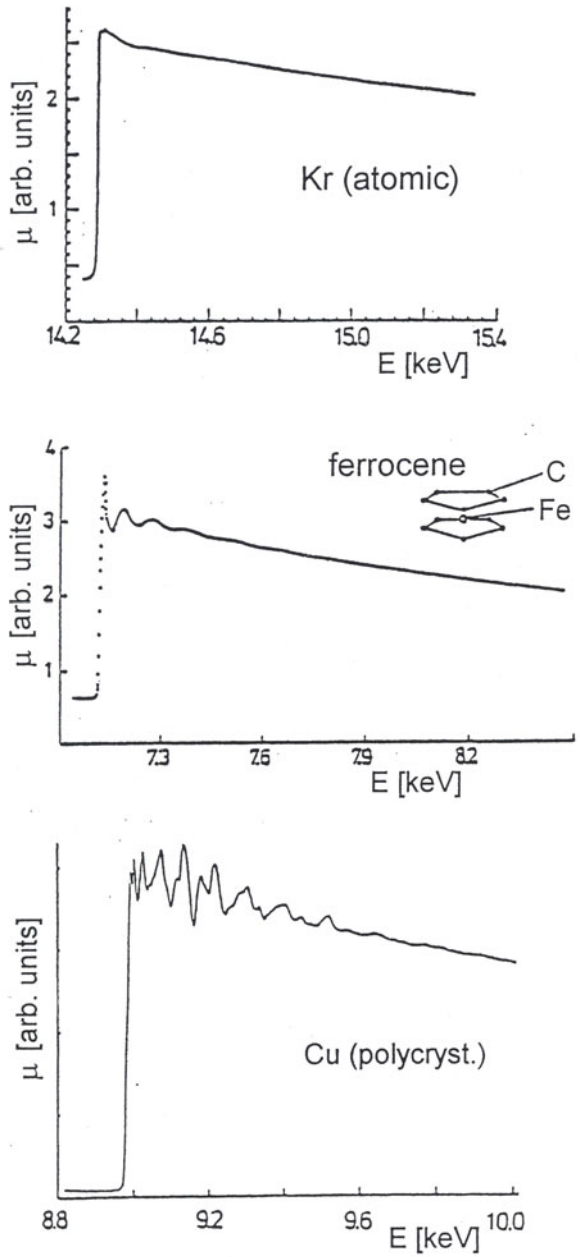
Advantages:

- Type of central atom can be selected
- Neighboring atoms can be identified
- Especially useful for dilute systems

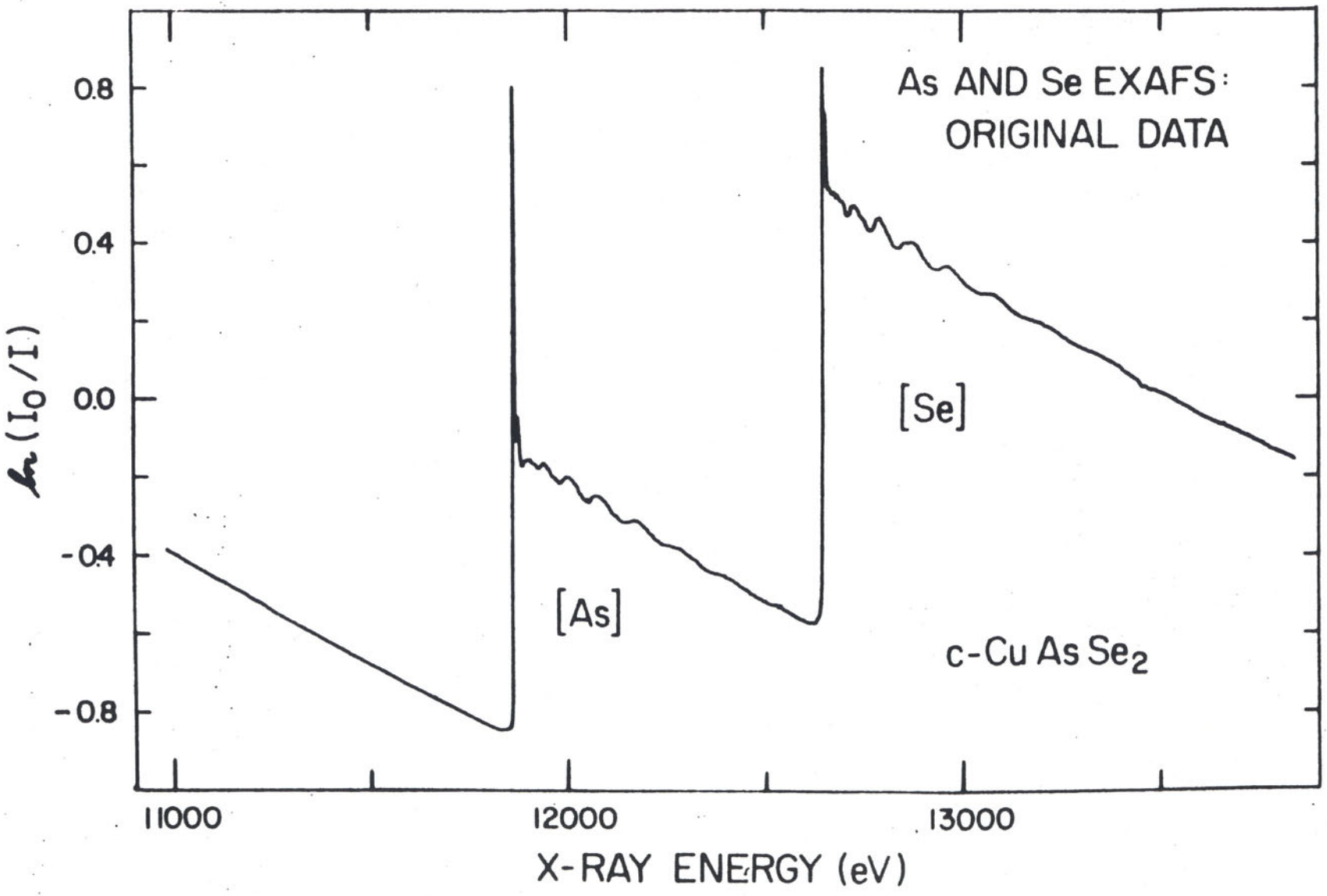
Samples:

- Crystalline and amorphous materials
- Surfaces
- Liquids
- Molecular gases

K-Kanten: Beispiele



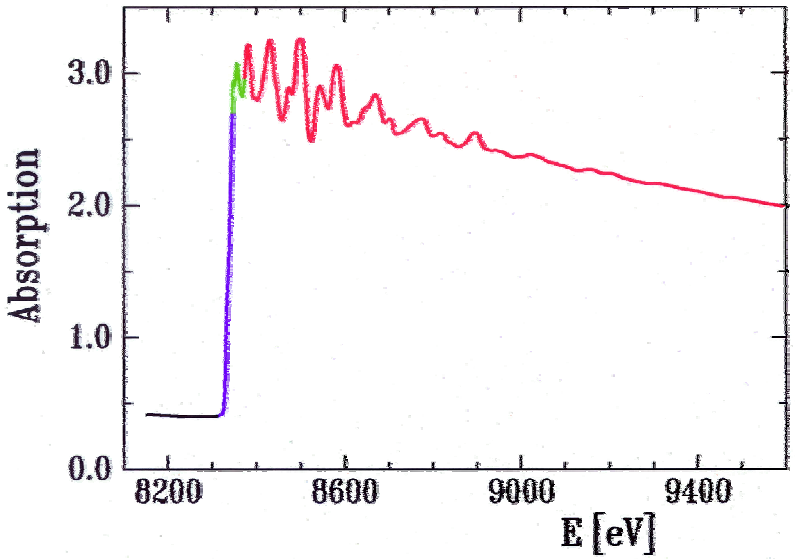
R. Frahm, Univ. of Duesseldorf



As and Se X-Ray Absorption Edges in c-$CuAsSe_2$: Original Data.

Sally Hunter; SSRL, ~1975

Absorption spectrum of Ni metal



Exact edge position ⇒ Valence state of the absorbing atoms

Near edge structure (XANES) ⇒ Bond angles

Extended structure (EXAFS) ⇒ Atomic distances
⇒ Coordination numbers
⇒ Identification of neighboring atoms

R. Frahm
Düsseldorf

MOLECULAR ENVIRONMENTAL SCIENCE (MES)

Objective: Provide information on natural and man-made waste forms.

- Chemical & Physical Forms (Speciation).
- Spatial Distribution.
- Reactivity.

Fundamental understanding of the complex molecular-scale environmental processes, both chemical& biological, that affect the stability, transformations, mobility and toxicity of contaminant species.

Molecular Environmental Science and Synchrotron Light Sources

Who cares about the distances between atoms?

Just about everyone should, including your next door neighbor, because such distances define molecular structure which in turn defines function or properties in natural materials, including those occurring in the environment and In living cells. The molecular form or speciation of environmental contaminants, such as chromium, arsenic, lead, uranium, or plutonium, determines their toxicity and bioavailablilty.

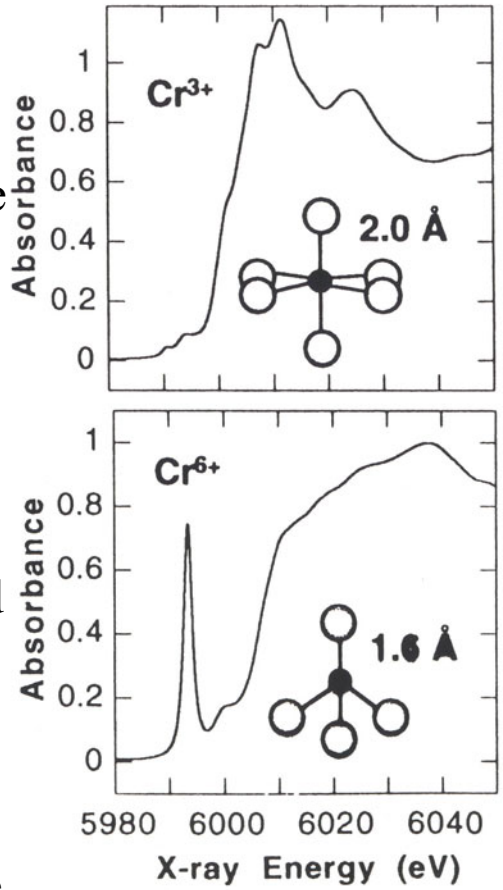
Molecular Environmental Science

• A new multidisciplinary field that has evolved over the past five years In response to the growing need to understand chemical and biological processes affecting environmental contaminants.

• Main objective Is to provide information on the types, spatial distribution, and reactivity of contaminant species.

Synchrotron Light Sources

Now play a very Important role In environmental science because the extremely intense x-rays from these sources are needed to detect and characterize the chemical and physical distributions of environmental contaminants.



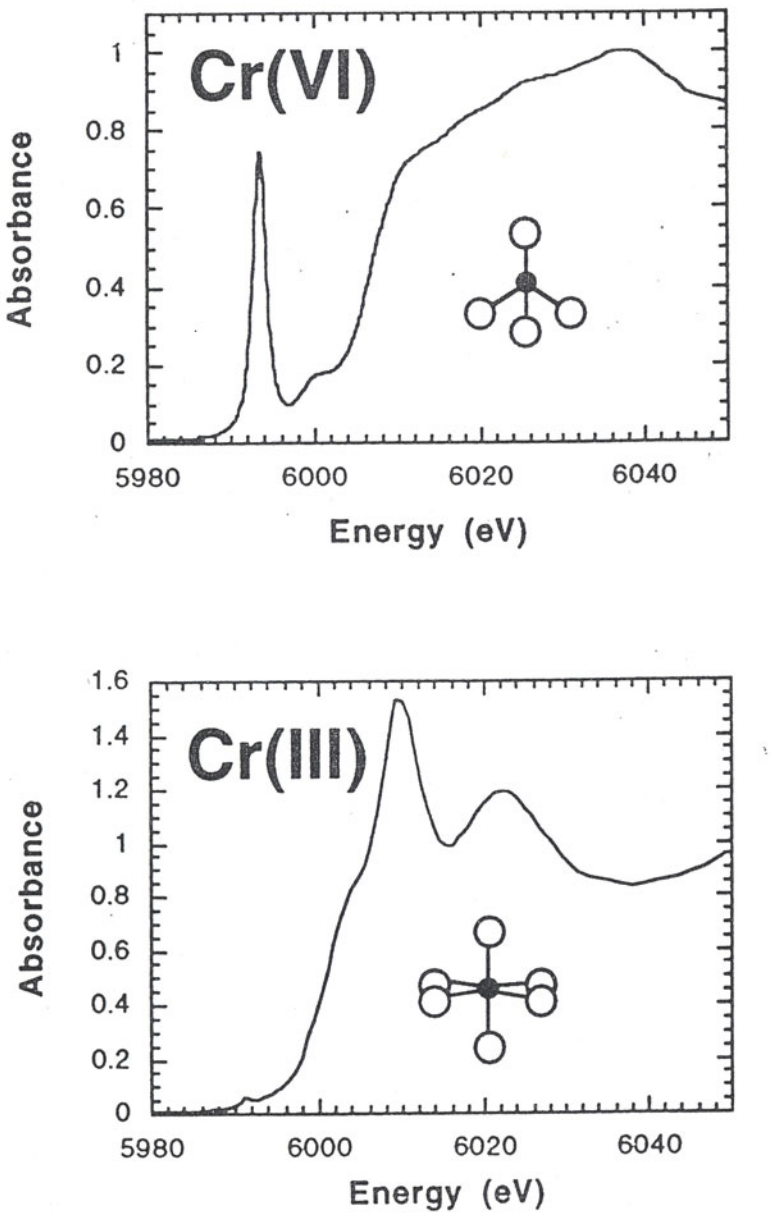
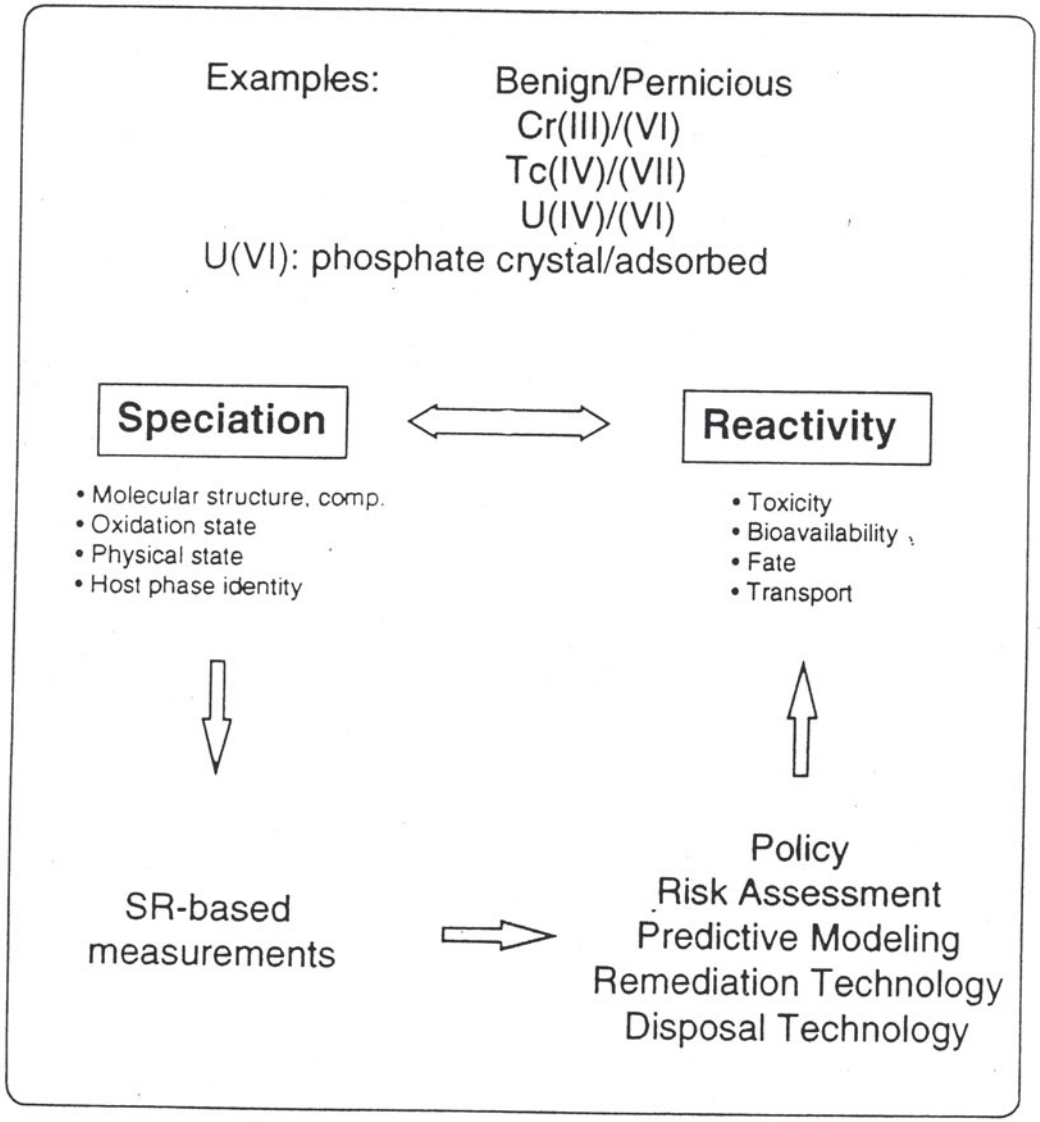


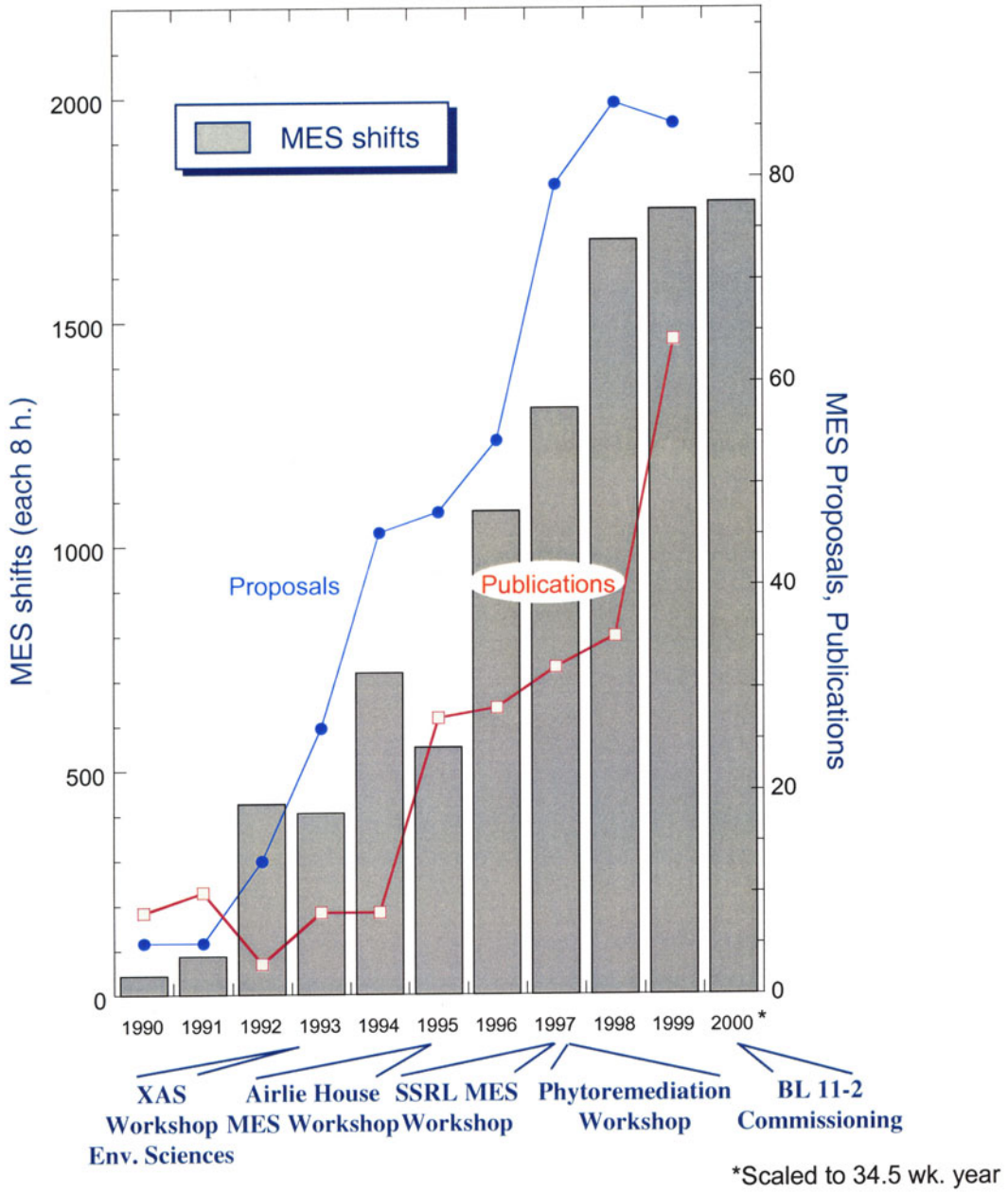
Fig. 7; EXAFS spectrum of Cr (VI) and Cr (III) illustrating the ability to identify oxidation states

Speciation of Contaminants



Speciation of contaminants & the role of synchrotron radiation

Growth of Molecular Environmental Science Activities at SSRL




The SSRL
Crystal
Mounting
Robot