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The role of XAFS in advancing the frontiers of molecular environmental science

Donald L. Sparks
University of Delaware Newark, Delaware, USA
dlsparks@udel.edu

One of the most widely used synchrotron-based spectroscopic techniques is x-ray absorption fine structure spectroscopy (XAFS). XAFS can be used to study most elements in crystalline or non-crystalline solid, liquid or gaseous states over a concentration range of a few mg/L to the pure element. XAFS can be used to probe structural sites ranging from those in crystals and glasses to those at interfaces such as the mineral/water interface. With third-generation synchrotron light sources that provide X-ray energies ranging from the infrared to the hard x-ray region, higher flux and more intense brightness, beamline optics that produce microfocused beams for spectromicroscopy and imaging studies, and state-of-the-art detectors, important advances in many scientific areas will occur over the next decade.

One of the major advantages of XAFS, particularly if one wants to simulate natural conditions in the environment, is that one can study reactions in the presence of water *(in situ)* This is a major advantage over many other molecular scale techniques, which are *ex-situ*, often requiring drying of the sample material, placing it in an ultra-high vacuum (UHV), heating the sample or employing particle bombardment. Such conditions can alter the sample, creating artifacts, and do not simulate most natural environmental conditions. It is especially important to study environmental reactions and processes in water as it is the principal medium of transport of inorganic and organic species, and biochemical reactions take place in aqueous media and across biological membranes that are water based. XAFS is an element specific, bulk method that yields information about the local structural and compositional environment of an absorbing atom. It “sees” only the 2 or 3 closest shells of neighbors around an absorbing atom due to the short electron mean free path in most substances. Using XAFS, one can ascertain important chemical information such as the oxidation state, information about next nearest neighbors, bond distances and coordination numbers.

Over the past decade, the use of XAFS to study important environmental reactions and processes has contributed to major advances in the environmental and earth sciences. Significant advances have occurred in determining the speciation and reaction mechanisms of metals, oxyanions, radionuclides, and microbes in soil and water environments. These frontiers in molecular environmental science have major impacts on environmental remediation, development of predictive models, and bioavailability and risk assessments. This presentation will focus on principles of XAFS and its application to: elucidating metal sorption/release kinetics and mechanisms at mineral/water and mineral/microbe interfaces, speciating metal and metalloid contaminants in soils and plants, and investigating humic substance-metal complexation on mineral surfaces.