

THEORETICAL INTERPRETATION OF XANES SPECTRA

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X-ray absorption near edge spectroscopy (XANES) is used at the Synchrotron Radiation Center (SRC) to probe a variety of samples. Our recent research has included examining shells (abalone and nacre), proteins (prion protein and amyloid), and bone. The spectrum produced by each of these samples provides information about the chemical and structural composition of the molecules making up the samples.

In theory, the spectra should be able to be decomposed into building blocks, that is, the chemical bonds that exist within the sample being examined. Yet, since each of the samples we are examining has complex chemical structures, the actual decomposition of the spectra is quite difficult and has a great deal of uncertainty built into the process, peak fitting and assignment for example.

Interpreting the XANES data with theoretical models of the system under analysis may eliminate some of the uncertainty and allow a better understanding of the system structure. FEFF, a molecular modeling code, simulates a XANES spectrum of the molecule based upon a user-generated input file, that includes the atomic positions, potentials, multiple scattering path length, cluster size, the type of exchange potential to be used, etc.

FEFF was originally created to do extended x-ray-absorption fine structure (EXAFS) simulations and was extended to XANES for crystalline inorganic molecules. Using FEFF to model organic systems pushes the limits of the code, thus a part of our study determines whether FEFF can be used on organic molecules in the soft x-ray region.

Before venturing into simulations of C spectra from complex organic molecules, we examined the simpler, biologically relevant minerals calcite and aragonite. We present a comparison between the spectra created by FEFF for these molecules and XANES experimental data acquired at the SRC. We found that FEFF is unable to reproduce accurate peak intensity or absolute energy positions, but can produce spectra that resemble experimental spectra and distinguishes calcite from aragonite. In conclusion, while FEFF can be used to distinguish systems, additional theories and models seem to be needed in order to fully describe and simulate XANES spectra of complex organic and inorganic molecules.