Structure Determination using High Throughput XAS and Data Mining

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Seeing the structure of materials on an atomistic level and visualizing the changes during a chemical process is essential in understanding materials functionality, and ultimately, in the concept of rational materials design. Core level spectroscopy with its sensitivity to hybridization and local symmetry is an ensemble averaging technique which has the potential to provide this visualization; in contrast to most microscopic techniques, sample preparation is relatively easy, the measurements fast, and most importantly, due to the ensemble probing character, the observed structure changes can be easily correlated with the functional behavior of the system.

Using the example of a ZnO/TiO_2 water splitting system we will show how near edge data from Zn and Ti can be combined with theoretical calculations of the absorption spectra to develop a structural model of the system. A data mining method is key to this approach; using the database entries of all known Zn-Ti-O structures, the absorptions spectra for all unique sites of these structures can be calculated and compared with the measured spectra. To ensure reliability and efficiency of the simulations and the "fitting algorithm", a large number of ZnO/TiO_2 systems is characterized as model system and compared with the simulations. In other words, the model systems are used to train a neural network in a "deep learning approach".

This new approach is extremely powerful but requires hundreds to thousands of calculations and measurements. In a third part of the talk we will discuss the various requirements on beamline, data acquisition system, and data analysis pipeline. We will also start the discussion the needs of standardization, quality control and data exchange through databases.