Joerg Prietzel:

Synchrotron-based X-ray Absorption Near Edge Structure (XANES) spectroscopy: A powerful tool to assess the speciation and cycling of important bioelements (e.g. S, P, Ca) in soils and other environmental samples

Abstract:

Environmental effects of nutrient or noxious elements in soils are often dependent on their oxidation state or binding form. Therefore, in soil science and other environmental sciences (e.g. geology, biology, agronomy) besides knowledge on total concentrations of a particular element under study, additionally knowledge on its binding forms in the investigated soil or environment is important. Traditional wet chemical methods of soil analysis most often allow only for a operationally-defined estimation rather than exact quantification of the respective amounts of different forms of a given bioelement in soils.

During the recent decades, synchrotron-based X-ray absorption spectroscopy methods, namely X-ray absorption near-edge structure (XANES) spectroscopy has emerged as a powerful tool for the identification and quantification of different binding forms of various bioelements with relevance in soils and other environments. However, application of XANES spectroscopy in soil science is particularly challenging, because soils compared to well-defined materials such as alloys, stones and rocks are often characterized by low concentrations of the element of interest. Moreover, the composition of soils often is poorly defined or even unknown, which complicates the selection of appropriate reference compounds for spectrum deconvolution and/or spectrum deconvolution itself.

In my talk, I will present several studies which demonstrate how synchrotron-based K-edge XANES spectroscopy can be used to reveal the speciation and cycling of various bioelements in soils, forest, and rangeland ecosystems. The examples include (i) studies on sulfur (S) and iron (Fe), which most often in soils are present in different oxidation states, depending on soil water saturation. Moreover, I will present (ii) studies on phosphorus (P) speciation in forest, rangeland and glacier forefield soils. Application of P K-edge XANES spectroscopy on soil samples is complicated, because soil P contents generally are low and P in soils is almost entirely present in only one single (+V) oxidation state. Spectral feature differences among different P forms in soils therefore often are not prominent and sometimes even absent. Finally, I will present novel results of (iii) a recent study on Ca speciation in forest soils. Here, particular binding properties of divalent Ca cations impose new methodological challenges for spectrum deconvolution.

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