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Thema
Kommission II: Bodenchemie

Korrelative Analyse biogeochemischer und struktureller Komplexizität im Boden

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Titel
To relate surface properties and surface elemental composition – Application of XPS in soil science

Abstract
Soil particles always are coated by thin layers (nm to µm) of predominantly organic compounds that form the interface between particle and pore space and govern soil functioning (e.g. liquid transport, sorption, respiration). Chemical modification of the surface layer can change surface properties such as wettability (quantified in terms of contact angle CA) with implications for e.g. liquid distribution and sorption capacity. This points to the importance to specifically analyze the coating's chemical composition in order to better understand soil functioning. The shallow analysis depth (max. 10 nm) indicates X ray photoelectron spectroscopy (XPS) as a suitable tool. Here, all elements with Z >= 3 will be identified by the binding energy of the photoelectrons emitted after irradiation of the surface by X rays. In sensu stricto only applicable to flat and smooth surfaces our results so far prove applicability of XPS as well to rough surfaces such as soil particles. For XPS no sample pre-treatment is needed, i.e. the surfaces analyzed are those governing e.g. CA and sorption. The relation between surface elemental composition and CA could be demonstrated within a soil chronosequence where the changes of surface element contents due to an increasing coating of the particles by organic compounds and microorganisms were correlated to increasing CA. The surface O/C ratio could be identified as a general parameter linking surface chemical composition and CA for a wide range of different materials including hydrophobized glass slides while the amount of non-polar C species was indicated to define CA. Artificially induced modifications of surface properties became visible by changes in the surface elemental composition. Gentle crushing of soil microaggregates (SMA) resulted in slightly increased N contents hinting on a preferred location of N compounds within SMA. Exposition to HCl gas to decrease soil pH or cleaning of quartz sand by HCl treatment resulted in addition of Cl and removal of Fe, respectively. However, due to its high surface sensitivity XPS measures the presence of C species on all surfaces exposed to the environment (adventitious carbon AC). AC was found to complicate the verification of sorption of small amounts of organic acids to montmorillonite, pointing on the necessity to estimate the influence of AC in certain cases. On the other hand, detection of AC indicates AC as a factor to be considered when discussing surface properties.