

## Visions for a Sustainable Planet

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Start

Browse by Section/Division of Interest

Author Index

267-7 Extended X-Ray Absorption Fine Structure Spectroscopic Determination of the Bonding Configuration of Orthophosphate Surface Complexes of Phosphate At the Goethite/Water Interface.

See more from this Division: S02 Soil Chemistry See more from this Session: Oxyanion Sorption and Speciation: I

Tuesday, October 23, 2012: 2:30 PM Duke Energy Convention Center, Room 207, Level 2



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It is known that soil chemical processes such as surface precipitation, adsorption and desorption of sorbed species are kinetically surface controlled and, thus, critically dependent on the surface speciation and reactivity. Solid-phase speciation of P on Fe- and AI- (hydr)oxides, such as goethite, ferrihydrite and boehmite, shows that bidentate binuclear and monodentate mononuclear structures are the predominant bonding configuration formed at these mineral surfaces (Tejedor-Tejedor & Anderson, 1990; Arai & Sparks, 2001; Khare et al. 2007). To the best of our knowledge, there are no reports in the literature where EXAFS spectroscopy was employed to obtain detailed structural information such as next nearest neighbor and bond distance on the P surface complexes formed at mineral surfaces.

We employed extended X-ray absorption fine structure (EXAFS) spectroscopy to determine the local atomic environment of P sorbed on the goethite surface. A range of orthophosphate concentrations was investigated in this study. The P concentrations employed in this study were chosen in order to obtain reaction products that would allow us to follow the transition from adsorption, at the lowest surface coverage (12.5 µmol m<sup>-2</sup>), to surface precipitates, at the highest P loading (100 µmol m<sup>-2</sup>).

Phosphorus K-edge EXAFS analyses were conducted at beamline X15B at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory in Upton, NY. EXAFS spectra were collected in fluorescence mode at the P K-edge at 2,150 eV via scans varying in energy from 2,100 to 2,750 eV.

The structural parameters were obtained through the fits of the sorption data to single and multiple scattering paths using Artemis. EXAFS analysis revealed a continuum between adsorption and surface precipitation, with bidentate mononuclear, bidentate binuclear and monodentate mononuclear surface complexes as well as surface precipitates forming at the goethite/water interface under the studied conditions. The coexistence of different surface complexes or the predominance of one sorption mechanism over others was directly related to surface loading.

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<< Previous Abstract | Next Abstract >>

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