

☒ Talk      ☐ Poster

## **Multi-modal, micro-spectroscopic speciation of legacy phosphorus in two U.S. mid-Atlantic agricultural soils**

Kathryn D. Szerlag<sup>1</sup>, Matthew G. Siebecker<sup>2</sup>, Fatemeh Izaditame<sup>3</sup>, Paul Northrup<sup>4</sup>, Ryan Tappero<sup>5</sup>, Donald L. Sparks<sup>6</sup>

<sup>1</sup> *Department of Soil and Crop Science, Texas A&M University, College Station, Texas, USA*

<sup>2</sup> *Department of Plant and Soil Science, Texas Tech University, Lubbock, Texas, USA*

<sup>3</sup> *Department of Geosciences, University of Texas, Dallas, USA*

<sup>4</sup> *Department of Geosciences, Stony Brook University, Stony Brook, New York, USA*

<sup>5</sup> *National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York, USA*

<sup>6</sup> *Department of Plant and Soil Science, University of Delaware, Newark, Delaware, USA*

*Author Email: kate.szerlag@ag.tamu.edu*

To understand phosphorus (P) mobility in agricultural soils and its potential environmental risk, it is essential to directly measure solid phase P speciation. Often, bulk P K-edge X-ray absorption near edge structure (XANES) spectroscopy followed by linear combination fitting (LCF) is utilized to determine the solid P phases in soil. However, this method may limit results to only a few major phases. Additionally, XANES spectra for different P species may have very similar features, leading to an over or underestimate of their contribution to LCF. Here, an improved P speciation by pairing multi-modal micro-focused X-ray fluorescence ( $\mu$ -XRF) mapping coupled with  $\mu$ -XANES analysis to directly speciate major and minor P phases on the micron scale is provided. We combined maps of both tender (P, S, Al, Si) and hard energy (Ca, Fe, Mn) elements to evaluate the elemental co-locations with P. To better account for uncertainty assigning XANES peaks to individual compounds, a more quantitative fingerprinting by “spectral feature analysis” was completed. With this analysis, an R-factor is reported for the fit. These results were compared to traditional LCF. Pre-edge fitting results revealed the presence of a two-component pre-edge feature for phosphate adsorbed to ferrihydrite. Additionally, phytate co-precipitated with ferrihydrite (Phytate-Fe-Cop) had a pre-edge feature, indicating direct association with Fe. Lastly, a unique P species associated with manganese oxide was identified in the soil via multi-modal mapping and  $\mu$ -XANES. These results allow for better prediction of P dissolution and mobility.