

The Role of Molecular Scale Investigations in Advancing the Frontiers of Contaminant Speciation and Bioavailability in Soils

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Environmental quality and sustainability is a concern worldwide. Contamination of soils and waters with metals, oxyanions, radionuclides, nutrients, and organic chemicals is the focus of research in a variety of fields including soil and environmental sciences and engineering. Ideally, one wants to understand environmentally important reactions and processes in natural systems at multiple scales to accurately predict the fate, transport, toxicity, and bioavailability of contaminants. In the past, most studies were conducted at larger scales such as the field and macroscopic scales. However, in the past decade, there have been major advances in the development and use of state-of-the-art in-situ analytical techniques that enable one to study an array of important reactions and processes at the molecular scale. In fact, a new interdisciplinary science has evolved based on the use of molecular scale approaches- molecular environmental science.

To delineate reaction mechanisms of contaminant reactions on soil minerals and in soils, it is advisable to couple macroscopic investigations with molecular scale studies. A large portion of this lecture will review advances in the employment of molecular scale in-situ analytical techniques (e.g., X-ray absorption and Fourier transform infrared spectroscopies) to speciate and elucidate contaminant retention/release mechanisms in soils and on soil components. Applications of these techniques to assess metal sorption/release, natural attenuation processes, and speciation of soil minerals and heterogeneous soils and poultry litter will be addressed. For example, using a variety of molecular and macroscopic scale techniques and approaches, it has been found that metals such as Co, Ni, and Zn can form metal hydroxide surface precipitates in soils over fairly rapid time scales, and that with time, mineral transformations occur which greatly enhances the sequestration of the metal. This could be an important natural attenuation mechanism, significantly affecting the bioavailability of metals. In recent years, micro-focused X-ray absorption spectroscopic and chemical mapping techniques allow one to speciate metal contaminants in soils over square micron scales. Examples and applications will be shown for Zn speciation in soils and for P speciation of chemically amended poultry litter material. Future research needs and directions will also be assessed.