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The value of a multi-scale, multi-tool approach in elucidating metal(loid) biogeochemistry in the environment

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The use of state-of-the-art, *in-situ* spectroscopic and microscopic techniques has greatly advanced our understanding of biogeochemical reactivity and speciation of metal(loids) at the mineral/water interface. These techniques enable one to make measurements at small spatial and rapid temporal scales and simulate natural environmental conditions. The use of small scale techniques in environmental research has resulted in a new multidisciplinary field of study that chemists, geochemists, and soil scientists are actively involved in – molecular environmental science. Molecular environmental science can be defined as the study of the chemical and physical forms and distribution of contaminants in soils, sediments, waste materials, natural waters, plants, and the atmosphere at the molecular level. The application of molecular environmental science tools to the study of metal(loid) biogeochemistry has resulted in major scientific breakthroughs. Undoubtedly, the molecular characterization of microenvironments and interfacial reactions will become increasingly significant in understanding the interactions between chemistry, physics, and biology in natural environments. There are a number of areas dealing with biogeochemistry of metal(loids) where the application of molecular environmental science is resulting in major frontiers. These include: speciation of contaminants, which is essential for understanding release mechanisms, spatial resolution, chemical transformations, toxicity, bioavailability, and ultimate impacts on human health; mechanisms of microbial transformations at mineral/metal(loid) interfaces; functional group distribution and structure of humic substances; mechanisms of trace metal interactions with humic substances; trace metal(loid) biochemistry at the plant/soil interface; development of predictive models; effective remediation and waste management strategies; and risk assessment. The use of these tools, coupled with computational modeling approaches, is rapidly advancing a number of research frontiers in geochemistry and related scientific fields. This paper will illustrate the application of a multi-scale, multi-tool approach to elucidate and model metal(loid) reactivity and processes at the mineral/water interface including: surface complexation and precipitation, mineral transformations, and oxidation-reduction dynamics.

Keywords: spatial and temporal scales, X-ray absorption spectroscopy, molecular modeling, metal(loid) reactivity, mineral/water interfacial processes, sorption