# 93rd Canadian Chemistry Conference and Exhibition

| 1191 | EN3 | 08:40 Tuesday AM | Room 201 B |
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**Integrating Spectroscopic, Kinetic, and Modeling Approaches to Elucidate the Mechanisms of Contaminant Interactions in Heterogeneous Natural Systems**

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The use of state-of-the-art, in-situ spectroscopic techniques has greatly advanced our understanding of biogeochemical reactivity and speciation of contaminants in natural, heterogeneous systems such as soils, sediments, and aquatic systems. These techniques enable one to make measurements at small spatial and rapid temporal scales and to simulate natural environmental conditions. 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 the biogeochemistry of contaminants where the application of molecular environmental science is resulting in major frontiers. These include: speciation of contaminants; 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, especially in real-time, and coupled with computational modeling approaches, is rapidly advancing a number of research areas in environmental chemistry and the geosciences. This paper will illustrate the application of a multi-scale, multi-tool approach to elucidate and model contaminant reactivity and processes in natural systems including: surface complexation, precipitation, and speciation, mineral transformations, and oxidation-reduction dynamics.

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**Bold text** denotes the presenting author. If present, * denotes the corresponding author and $ denotes the principal investigator.