

## **Biogeochemical and Molecular Mechanisms Controlling Contaminant Transformation in the Environment**

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Anthropogenic releases and changing environmental conditions lead to profound impact on the biogeochemical cycle of trace metals, such as mercury (Hg). Mercury can be methylated to form methylmercury (MeHg), which bioaccumulates in the food web, endangering humans and other biota. Since its inception 6 years ago, the Oak Ridge National Laboratory (ORNL) Science Focus Area (SFA) program has made substantial progress in fulfilling the original overarching objective of ***elucidating the mechanisms by which inorganic mercury (Hg) is transformed into MeHg at the sediment–water interface and the processes that determine net MeHg production at contaminated sites***. The program's progress has resulted in a number of groundbreaking insights and discoveries, including the discovery of the Hg methylation genes (*hgcAB*) and their organismal and environmental distribution, the dual functional role of DOM in Hg redox transformation, and the fact that certain anaerobic microorganisms are capable of using dissolved elemental Hg(0) for methylation.

Our efforts since the last review have led to the realization that exchange and feedback processes occurring at critical interfaces are key factors limiting our predictive understanding of net MeHg production in environmental systems. Critical interfaces connect different ecosystem compartments and subsystem components enabling exchange, feedback, and co-evolution. In the spring, this SFA will undergo DOE peer-review. The Renewal Proposal aims to generate new knowledge in three thrusts: microbial community dynamics; fundamental biogeochemical processes; and molecular scale interactions that control Hg speciation, bioavailability, and transformations at critical interfaces along the hydrologic transport pathway. Accomplishing these objectives will contribute to the SFA's 3-year goal of ***determining the fundamental mechanisms and environmental factors that control Hg biogeochemical transformations at critical interfaces in terrestrial and aquatic ecosystems***.

This system science program integrates hydrology, geochemistry, microbiology, and computational science, including molecular simulations, to investigate Hg behavior in environmental systems. The multidisciplinary and multiinstitutional program is supported by ORNL's core expertise in field-to-laboratory scale geochemistry and microbiology and its world-class neutron source and high-performance computing capabilities. Newly generated tools and knowledge will enable a deeper understanding of Hg and trace metal speciation and flux across critical interfaces, improving predictions of trace metal biogeochemical cycles in heterogeneous and multiscaled environmental systems locally and globally.