*DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE*

*SEMINAR SERIES*

*SPRING 2024*

WEDNESDAY, APRIL 3

TIERNAN HALL – LECT. HALL 2

1:00PM-2:20PM

# **GUEST SPEAKER**

Dr. Ian Bourg

Associate Professor

Civil and Environmental Engineering

Princeton University

**TOPIC**

Molecular dynamics simulation predictions of the partitioning of PFAS between water, air, and mineral surfaces

**ABSTRACT**

The tendency of per- and polyfluoroakyl substances (PFAS) to partition between water, air, and mineral surfaces is an important set of properties that impacts their fate and transport in natural systems. A key challenge associated with efforts to predict the associated partitioning coefficients is the need for accurate partitioning data for a wide variety of PFAS between many phases or interfaces and over a variety of chemical conditions. Molecular dynamics (MD) simulations have the potential to facilitate the generation of these data, but they have been applied only to a limited number of compounds and adsorbents. Here, we report MD simulations of the partitioning of a relatively wide variety of PFAS (including cationic, anionic, and zwitterionic compounds and PFAS precursors) at water-air and mineral-water interfaces in different aqueous chemistry conditions. Simulation results provide quantitative predictions of adsorption and partitioning coefficients and fundamental insight into the mechanisms that control these coefficients.

**BIO**

A person smiling for a picture

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Ian Bourg is an Associate Professor in Civil and Environmental Engineering at Princeton University. His group studies the properties of water at interfaces, with a particular emphasis on the impact of clay minerals on subsurface hydrology, soil mechanics, carbon dynamics, geochemistry, and contaminant fate and transport. He obtained a B.Eng. in Industrial Process Engineering from the National Institute for Applied Sciences in Toulouse in 1999 and a Ph.D. in Civil and Environmental Engineering from the University of California at Berkeley in 2004. He led a research group in the Earth Sciences Division at the Lawrence Berkeley National Laboratory until 2014 before joining the faculty at Princeton University in 2015.

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