Molecular dynamics simulation of mica wetting by water and organics

EMILY WEI-HSIN SUN[1], IAN C. BOURG[2]

[1]Civil and Environmental Engineering, Princeton University, Princeton, New Jersey, United States esun@princeton.edu
[2]Civil and Environmental Engineering, Princeton University, Princeton, New Jersey, United States bourg@princeton.edu

A fundamental understanding of confined wetting and multiphase flow is crucial for many natural and engineered systems. For example, soils keep an estimated 1440 Pg of soil organic carbon (SOC) from cycling to the atmosphere, and are therefore an immense potential source of greenhoouse gas in response to global climate change. The persistence of SOC has been linked to dynamic mechanisms of stabilization in mineral matrices. Physical and chemical features governing multiphase flow of water and organics in nano-scale mineral pores have been shown to impact soil water infiltration and aggregation, potentially important factors in SOC stability. However, the mechanisms behind these phenomena are poorly known.

An important knowledge gap is a mechanistic understanding of SOC arrangement on mineral surfaces, and the influence of SOC on wettability. Molecular dynamics (MD) simulations have shown significant promise in elucidating nano-scale organic solute phenomena at mineral interfaces such as absorption mechanisms, contact angles (CAs), and other multiphase flow properties in ideal systems. In this study, we carry out a series of MD simulations to probe water CAs on mica in the presence of organic molecules. We simulate an air bubble in a water-filled mica nano-pore with varying SOC proxy molecule concentrations and functionalities. We scale up these simulations to a large unconfined droplet in an attempt to bridge nano- and micro-scale CAs. These methods also allow us to examine mechanisms of interaction within thin water films near the mineral surface. We find that high concentrations of certain organics may influence the water wetting and aggregation behavior of mica.