# Influence of Sugar Molecules on Water Dynamics and Interactions in Clay Nanopores

STEPHEN M. GALDI [1], THALIA G. AOKI[1], LUDMILLA ARISTILDE[1*]

[1]Department of Biological and Environmental Engineering, College of Agriculture and Life Sciences, Cornell University (*correspondence: ludmilla@cornell.edu)

Waters and solutes trapped in soil nanopores provide for long-term storage of soil moisture and nutrients as well as long-term residence of pollutants. The application of molecular dynamics simulations has been widely adopted to investigate molecular diffusion in hydrated clay nanopores. Much attention has been devoted to the hydrodynamics of waters and cations in soil nanopores. However, little is known about the influence of the ubiquitous presence of organic molecules in soil nanopores on these hydrodynamic behaviors.

Of special interest is the dynamics in hydrated mineral nanopores populated by sugars, which are common organic substrates secreted by plant and microbial biota. Here we present findings from molecular dynamics simulations of a montmorillonite clay interlayer nanopore with increasing amounts of adsorbed glucose molecules (Figure 1). We captured sugar-influenced dynamic perturbations both in the hydration of the mineral surface and in the water-solute interaction networks. We interpreted these perturbations in light of resulting changes in water and solute diffusion determined in the simulated clay nanopore.

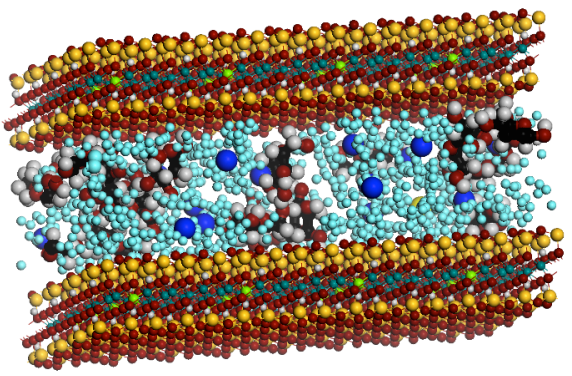

**Figure 1.** Snapshot of molecular dynamics-equilibrated systems with 0.1 M NaCl solution confined in a 20 Å-wide montmorillonite nanopore in the presence of 16 glucose molecules. Color legend: O (red), H (white), Si (yellow), dark green (Al), light green (Mg), Na (dark blue), water molecules (light blue).