Water Trapping Dynamics in Clay-Populated Smectite Nanopores: Experiments and Theory

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Smectite-type clay minerals play a critical role in the trapping of fluids within soil nanopores. The hydrodynamics of cation-saturated smectite interlayers is well documented. However, little is known about how the hydration behavior of smectite interlayer nanopores is influenced by small organic compounds. Here we applied a combination of experimental and theoretical techniques to probe the effects of carbohydrates, an important and abundant class of organic compounds in soils, on the hydration properties of montmorillonite, a prototypical smectite mineral. Specifically, we employed Fourier-transform infrared spectroscopy to monitor populations of exchangeable waters within the hydrated mineral aggregates. Water adsorption-desorption profiled were obtained to monitor relative water retention in the carbohydrate-populated montmorillonite samples in response to dehydration. We employed quantitative analysis of X-ray diffraction patterns to determine nanopore size distributions in the mineral aggregates subjected to *in situ* dehydration (Figure 1). We also performed molecular dynamics simulations to gain insights on the interfacial water dynamics in the absence and presence of carbohydrates. Our data collectively provide insights on how carbohydrates promote moisture retention in smectite nanopores by sustaining expanded nanopore pore size and facilitating water trapping at the mineral interface.

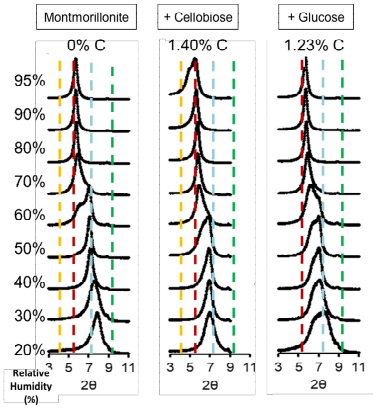

Figure 1. Moisture-dependent X-ray diffraction profiles of nanopore width of montmorillonite alone or loaded with cellobiose or glucose. The yellow, red, blue, and green dashed lines represent 1.87 nm, 1.56 nm, 1.3 nm, and 1.123 nm pore, respectively.